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Full List of Information

Provided By

Chemical Compounds DEEP PROFILING SERVICES

For Any Chemical Compound

Comprising C, H, N, O, S, F, Cl, Br, I, Si, P, and/or As.

https://www.cc-dps.com

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Property Information

Constant Thermo-Physicochemical, Thermodynamic, and Transport Properties

1. Absolute Entropy of Ideal Gas at 298.15 K and 1 bar
2. Acentric Factor
3. Critical Compressibility Factor
4. Critical Pressure
5. Critical Temperature
6. Critical Volume
7. Dipole Moment
8. Electron Affinity
9. Enthalpy (Heat) of Formation for Ideal Gas at 298.15 K
10. Enthalpy (Heat) of Fusion at Melting Point*
11. Flash Point
12. Gibbs Energy of Formation for Ideal Gas at 298.15 K and 1 bar
13. Heat (Enthalpy) of Vaporization at 298.15 K
14. Heat (Enthalpy) of Vaporization at Normal Boiling Point
15. Ionization Potential
16. Liquid Density at Normal Boiling Point
17. Liquid Molar Volume at 298.15 K
18. Lower Flammability Limit Temperature
19. Lower Flammability Limit Volume Percent
20. Magnetic Susceptibility
21. Net Standard State Enthalpy (Heat) of Combustion at 298.15 K**
22. Normal Boiling Point
23. Parachor
24. Polarizability
25. Radius of Gyration
26. Refractive Index
27. Solubility Parameter at 298.15 K
28. Standard State Absolute Entropy at 298.15 K and 1 bar
29. Standard State Enthalpy (Heat) of Formation at 298.15 K and 1 bar
30. Standard State Gibbs Energy of Formation at 298.15 K and 1 bar
31. Upper Flammability Limit Temperature
32. Upper Flammability Limit Volume Percent
33. van der Waals Area
34. van der Waals Reduced Volume

*Available only for the chemical compounds consisting of C, H, N, O, and S atoms.
**Available only for the chemical compounds consisting of C, H, N, O, S, F, Cl, Br, and I atoms.

Temperature Dependent Thermo-Physicochemical, Thermodynamic, and Transport Properties

1. Heat Capacity of Ideal Gas

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2. Heat Capacity of Liquid
3. Heat of Vaporization
4. Liquid Density
5. Second Virial Coefficient
6. Surface Tension
7. Thermal Conductivity of Gas
8. Thermal Conductivity of Liquid
9. Vapor Pressure of Liquid
10. Viscosity of Gas
11. Viscosity of Liquid

Pharmaceutical Properties

1. Activity Score for GPCR Ligands
2. Activity Score for Ion Channel Modulators
3. Activity Score for Kinase Inhibitors
4. Activity Score for Nuclear Receptor Ligands
5. Drug-Likeness
6. Ghose-Crippen Molar Refractivity
7. Ghose-Crippen Octanol-Water Partition Coeff. (logP)
8. Lipinski Alert Index
9. LogP (Octanol-Water Partition Coefficient)
10. LogS (Water Solubility)
11. Moriguchi Octanol-Water Partition Coeff. (logP)
12. Number of Acceptor Atoms for H-bonds (N,O)
13. Number of Donor Atoms for H-bonds (N,O)

Physical Property Datafile (Downloadable IK-Cape File) for Importing to Process Simulation Software (e.g., Aspen Plus) Containing:

1. Molecular Weight
2. Acentric Factor
3. Critical Compressibility Factor
4. Critical Temperature
5. Critical Pressure
6. Critical Volume
7. Dipole Moment
8. Heat of Melting at Normal Melting Point
9. Volume at Standard Conditions
10. Normal Boiling Point (1 atm)
11. Radius of Gyration
12. Standard Entropy (Vapor)
13. Standard Entropy (Liquid)
14. Standard Entropy (Solid)
15. Standard Heat of Formation (Vapor)

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16. Standard Heat of Formation (Liquid)
17. Standard Heat of Formation (Solid)
18. Standard Free Energy of Formation (Vapor)
19. Standard Free Energy of Formation (Liquid)
20. Standard Free Energy of Formation (Solid)
21. Parachor
22. Heat of Vaporization at Normal Boiling Point
23. Heat Capacity of Ideal Gas
24. Heat Capacity (Vapor, Liquid)
25. Heat of Vaporization
26. Density (Liquid)
27. Surface Tension
28. Thermal Conductivity (Vapor, Liquid)
29. Vapor Pressure
30. Viscosity (Vapor, Liquid)
31. Second Virial Coefficient
32. Refractive Index, Na-D-Line
33. Octanol/Water Partition Coefficient
34. Solubility within Water
35. Heat of Formation (Vapor, Liquid)
36. Enthalpy (Vapor, Liquid)
37. Entropy (Vapor, Liquid)
38. Gibbs Energy (Vapor, Liquid)
39. Gibbs Energy of Formation (Vapor, Liquid)

Properties Provided Based on Other Existing Methods Additionally for Comparison

1.	Acentric Factor	Gani[1]
2.	Critical Compressibility Factor	Joback[2], Gani[1]
3.	Critical Pressure	Joback[2], Gani[1]
4.	Critical Temperature	Joback[2], Gani[1]
5.	Critical Volume	Joback[2], Gani[1]
6.	Enthalpy (Heat) of Formation for Ideal Gas at 298.15 K	Joback[2], Gani[1]
7.	Enthalpy (Heat) of Fusion at Melting Point	Joback[2]
8.	Gibbs Energy of Formation for Ideal Gas at 298.15 K and 1 bar	Joback[2], Gani[1]
9.	Heat (Enthalpy) of Vaporization at Normal Boiling Point	Joback[2]
10.	Liquid Molar Volume at 298.15 K	Gani[1]
11.	Normal Boiling Point	Joback[2], Gani[1]
12.	Heat Capacity of Ideal Gas	Joback[2]
13.	Heat Capacity of Liquid	Bondi[3]
14.	Heat of Vaporization	Watson[4]
15.	Liquid Density	Rackett[5], Gunn-Yamada[6]
16.	Second Virial Coefficient	Mccann[7]
17.	Surface Tension	Brock-Bird[8], Miller[9]

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18.	Thermal Conductivity of Gas	Misic-Thodos[10], Mod-Eucken[11]
19.	Thermal Conductivity of Liquid	Sato-Riedel[12]
20.	Vapor Pressure of Liquid	Riedel[13]
21.	Viscosity of Gas	Reichenberg[14]
22.	Viscosity of Liquid	Joback[2], Letsou-Stiel[15], Orrick-Erbar[16]

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Spectroscopic Analyses

IR (Infrared) Spectra

1. IR Chart with User Interface
2. IR Frequency & Intensity Data Table
3. IR Datafile (Downloadable JDX File)
4. IR Vibrational 3D Frequency Animation

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NMR (Nuclear Magnetic Resonance) Spectra

1. H NMR and C NMR Chart with User Interface
2. H NMR and C NMR Shielding Data Table

VCD (Vibrational Circular Dichroism) Spectra

1. VCD Chart with User Interface
2. VCD Frequency & Intensity Data Table

Quantum Chemical Information

Quantum Chemical Visualization Properties

1. Optimized 3D Structure Data (Downloadable MOL File)
2. Optimized 3D Structure Image
3. Optimized 3D Structure Interactive Visualization
4. Optimized 3D Structure Bond Length and Bond Angle Measurement
5. Vibrational Frequency Data
6. Vibrational Frequency 3D Image
7. Vibrational Frequency Interactive Visualization
8. Vibrational Frequency 3D Animation
9. Molecular Orbitals 2D Image
10. Molecular Orbitals 3D Image
11. Molecular Orbitals Interactive Visualization

Quantum Chemical Computation Result File (Downloadable FCHK File)

Quantum Chemical Computation Data

1. Number of Atoms
2. Charge
3. Spin Multiplicity
4. Number of Electrons
5. Number of Alpha Electrons
6. Number of Beta Electrons
7. Number of Basis Functions
8. Number of Contracted Shells
9. Highest Angular Momentum
10. Largest Degree of Contraction
11. number of primitive shells

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12. Virial Ratio
13. Total Energy
14. Atomic Numbers
15. Nuclear Charges
16. Cartesian Coordinate
17. Cartesian Gradient
18. Cartesian Force Constants
19. Dipole Moment
20. Mulliken Charges
21. Integer Atom Types
22. MM (Molecular Mechanics) Charges
23. Integer Atomic Weights
24. Real Atomic Weights
25. Atom Residue Info
26. Atom Fragment Info
27. Atom Residue Num
28. Nuclear Spins
29. Nuclear ZEFF (Effective Charge)
30. Nuclear QMom (Quadrupole Moment)
31. Nuclear GFac (Magnetic Moment)
32. MicOpt
33. Constraint Structure
34. ONIOM Charges
35. ONIOM Spin Multiplicities
36. Atom Layers
37. Atom Modifiers
38. Integer Atom Modified Types
39. Link Atoms
40. Atom Modified MM (Molecular Mechanics) Charges
41. Link Distances
42. NBond (Formal Number of Bonds)
43. IBond Connectivity Information (Integer)
44. RBond Connectivity Information (Real)
45. Shell Types
46. Number of Primitives Per Shell
47. Shell to Atom Map
48. Primitive Exponents
49. Contraction Coefficients
50. Contraction Coefficients for P Portion of S=P Shells
51. Coordinates of Each Shell
52. Alpha Orbital Energies
53. Beta Orbital Energies
54. NMR Shielding
55. Spin-Rotation Tensors
56. QEq (Charge Equilibration) Coupling Tensors
57. Optimization Point: 1 Results for Each Geometry

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58. Optimization Point: 1 Geometries
59. Optimization Point: 1 Gradient at Each Geometry
60. Optimization Number of Geometries

Quantum Chemical Descriptors

1. No. of Occupied Electronic Levels
2. No. of Occupied Electronic Levels / No. of Atoms
3. HOMO-1 Energy
4. HOMO Energy
5. LUMO Energy
6. LUMO+1 Energy
7. HOMO - LUMO Energy Gap
8. Min Nucleophilic Reactivity Index (S)
9. Max Nucleophilic Reactivity Index (S)
10. Average Nucleophilic Reactivity Index (S)
11. Min Nucleophilic Reactivity Index (N)
12. Max Nucleophilic Reactivity Index (N)
13. Average Nucleophilic Reactivity Index (N)
14. Min Nucleophilic Reactivity Index (C)
15. Max Nucleophilic Reactivity Index (C)
16. Average Nucleophilic Reactivity Index (C)
17. Min Nucleophilic Reactivity Index (O)
18. Max Nucleophilic Reactivity Index (O)
19. Average Nucleophilic Reactivity Index (O)
20. Min Electrophilic Reactivity Index (S)
21. Max Electrophilic Reactivity Index (S)
22. Average Electrophilic Reactivity Index (S)
23. Min Electrophilic Reactivity Index (N)
24. Max Electrophilic Reactivity Index (N)
25. Average Electrophilic Reactivity Index (N)
26. Min Electrophilic Reactivity Index (C)
27. Max Electrophilic Reactivity Index (C)
28. Average Electrophilic Reactivity Index (C)
29. Min Electrophilic Reactivity Index (O)
30. Max Electrophilic Reactivity Index (O)
31. Average Electrophilic Reactivity Index (O)
32. Min 1-Electron Reactivity Index (S)
33. Max 1-Electron Reactivity Index (S)
34. Average 1-Electron Reactivity Index (S)
35. Min 1-Electron Reactivity Index (N)
36. Max 1-Electron Reactivity Index (N)
37. Average 1-Electron Reactivity Index (N)
38. Min 1-Electron Reactivity Index (C)
39. Max 1-Electron Reactivity Index (C)
40. Average 1-Electron Reactivity Index (C)

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41. Min 1-Electron Reactivity Index (O)
42. Max 1-Electron Reactivity Index (O)
43. Average 1-Electron Reactivity Index (O)
44. Max Net Atomic Charge (S)
45. Min Net Atomic Charge (S)
46. Max Net Atomic Charge (N)
47. Min Net Atomic Charge (N)
48. Max Net Atomic Charge (C)
49. Min Net Atomic Charge (C)
50. Max Net Atomic Charge (O)
51. Min Net Atomic Charge (O)
52. Max Net Atomic Charge (H)
53. Min Net Atomic Charge (H)
54. Max Net Atomic Charge
55. Min Net Atomic Charge
56. Total Molecular Dipole
57. Total Point Charge Comp. (Molecular Dipole)
58. Total Hybridization Comp. (Molecular Dipole)
59. Image of The Onsager-Kirkwood Solvation Energy
60. Total Molecular Surface Area
61. Partial Positive Surface Area
62. Partial Negative Surface Area
63. Difference in Charged Partial Surface Areas (PPSA1-PNSA1)
64. Fractional Partial Positive Surface Area (PPSA-1/TMSA)
65. Fractional Partial Negative Surface Area (PNSA-1/TMSA)
66. Weighted Partial Positive Surface Area (PPSA1*TMSA/1000)
67. Weighted Partial Negative Surface Area (PNSA1*TMSA/1000)
68. Total Charge Weighted Partial Positive Surface Area
69. Total Charge Weighted Partial Negative Surface Area
70. Difference in Charged Partial Surface Areas (PPSA2-PNSA2)
71. Fractional Total Charge Weighted Partial Positive Surface Area (PPSA-2/TMSA)
72. Fractional Total Charge Weighted Partial Negative Surface Area (PNSA-2/TMSA)
73. Weighted Total Charge Weighted Partial Positive Surface Area (PPSA2*TMSA/1000)
74. Weighted Total Charge Weighted Partial Negative Surface Area (PNSA2*TMSA/1000)
75. Atomic Charge Weighted Partial Positive Surface Area
76. Atomic Charge Weighted Partial Negative Surface Area
77. Difference in Charged Partial Surface Areas (PPSA3-PNSA3)
78. Fractional Atomic Charge Weighted Partial Positive Surface Area (PPSA-3/TMSA)
79. Fractional Atomic Charge Weighted Partial Negative Surface Area (PNSA-3/TMSA)
80. Weighted Atomic Charge Weighted Partial Positive Surface Area (PPSA3*TMSA/1000)
81. Weighted Atomic Charge Weighted Partial Negative Surface Area (PNSA3*TMSA/1000)
82. Relative Positive Charge (Most Positive Charge / Total Positive Charge)
83. Relative Positive Charged Surface Area (Most Positive Surface Area * RPCG)
84. Relative Negative Charge (Most Negative Charge / Total Negative Charge)
85. Relative Negative Charged Surface Area (Most Negative Surface Area * RNCG)
86. H-Donors Surface Area

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87. Fractional H-Donors Surface Area (HDSA/TMSA)
88. H-Acceptors Surface Area
89. Fractional H-Acceptors Surface Area (HASA/TMSA)
90. H-Bonding Surface Area
91. Fractional H-Bonding Surface Area (HBSA/TMSA)
92. H-Donors Charged Surface Area
93. Fractional H-Donors Charged Surface Area (HDCA/TMSA)
94. H-Acceptors Charged Surface Area
95. Fractional H-Acceptors Charged Surface Area (HACA/TMSA)
96. H-Bonding Charged Surface Area
97. Fractional H-Bonding Charged Surface Area (HBCA/TMSA)
98. Min(N_H-Acceptor, N_H-Donor)
99. Count Of H-Acceptor Sites
100. Count Of H-Donor Sites
101. HA Dependent H-Donors Surface Area-1
102. HA Dependent H-Donors Surface Area-1/TMSA
103. HA Dependent H-Donors Surface Area-2
104. HA Dependent H-Donors Surface Area-2/TMSA
105. HA Dependent H-Donors Surface Area-2/Sqrt(TMSA)
106. HA Dependent H-Donors Charged Surface Area-1
107. HA Dependent H-Donors Charged Surface Area-1/TMSA
108. HA Dependent H-Donors Charged Surface Area-2
109. HA Dependent H-Donors Charged Surface Area-2/TMSA
110. HA Dependent H-Donors Charged Surface Area-2/Sqrt(TMSA)
111. H-Acceptors Surface Area-1
112. H-Acceptors Surface Area-1/TMSA
113. H-Acceptors Surface Area-2
114. H-Acceptors Surface Area-2/TMSA
115. H-Acceptors Surface Area-2/Sqrt(TMSA)
116. H-Acceptors Charged Surface Area-1
117. H-Acceptors Charged Surface Area-1/TMSA
118. H-Acceptors Charged Surface Area-2
119. H-Acceptors Charged Surface Area-2/TMSA
120. H-Acceptors Charged Surface Area-2/Sqrt(TMSA)
121. Min Atomic Orbital Electronic Population
122. Max Atomic Orbital Electronic Population
123. Max Bond Order (Sigma-Sigma)
124. Max Bond Order (Pi-Pi)
125. Max Bond Order (Sigma-Pi)
126. Min Valency (S)
127. Max Valency (S)
128. Average Valency (S)
129. Min (>0.1) Bond Order (S)
130. Max Bond Order (S)
131. Average Bond Order (S)
132. Min Valency (N)

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133. Max Valency (N)
134. Average Valency (N)
135. Min (>0.1) Bond Order (N)
136. Max Bond Order (N)
137. Average Bond Order (N)
138. Min Valency (C)
139. Max Valency (C)
140. Average Valency (C)
141. Min (>0.1) Bond Order (C)
142. Max Bond Order (C)
143. Average Bond Order (C)
144. Min Valency (O)
145. Max Valency (O)
146. Average Valency (O)
147. Min (>0.1) Bond Order (O)
148. Max Bond Order (O)
149. Average Bond Order (O)
150. Min Valency (H)
151. Max Valency (H)
152. Average Valency (H)
153. Min (>0.1) Bond Order (H)
154. Max Bond Order (H)
155. Average Bond Order (H)
156. Full Molecular Orbitals Energies (HOMO, HOMO-1, HOMO-2..., LUMO, LUMO+1, LUMO+2...)

Electrostatic Descriptors

1. Max Partial Charge (S)
2. Min Partial Charge (S)
3. Max Partial Charge (C)
4. Min Partial Charge (C)
5. Max Partial Charge (N)
6. Min Partial Charge (N)
7. Max Partial Charge (O)
8. Min Partial Charge (O)
9. Max Partial Charge (H)
10. Min Partial Charge (H)
11. Max Partial Charge
12. Min Partial Charge
13. Polarity Parameter
14. Polarity Parameter/Square Distance
15. Topographic Electronic Index (All Pairs)
16. Topographic Electronic Index (All Bonds)
17. Total Molecular Surface Area
18. Partial Positive Surface Area
19. Partial Negative Surface Area

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20. Difference in Charged Partial Surface Areas (PPSA1-PNSA1)
21. Fractional Partial Positive Surface Area (PPSA-1/TMSA)
22. Fractional Partial Negative Surface Area (PNSA-1/TMSA)
23. Weighted Partial Positive Surface Area (PPSA1*TMSA/1000)
24. Weighted Partial Negative Surface Area (PNSA1*TMSA/1000)
25. Total Charge Weighted Partial Positive Surface Area
26. Total Charge Weighted Partial Negative Surface Area
27. Difference In Charged Partial Surface Areas (PPSA2-PNSA2)
28. Fractional Total Charge Weighted Partial Positive Surface Area (PPSA-2/TMSA)
29. Fractional Total Charge Weighted Partial Negative Surface Area (PNSA-2/TMSA)
30. Weighted Total Charge Weighted Partial Positive Surface Area (PPSA2*TMSA/1000)
31. Weighted Total Charge Weighted Partial Negative Surface Area (PNSA2*TMSA/1000)
32. Atomic Charge Weighted Partial Positive Surface Area
33. Atomic Charge Weighted Partial Negative Surface Area
34. Difference in Charged Partial Surface Areas (PPSA3-PNSA3)
35. Fractional Atomic Charge Weighted Partial Positive Surface Area (PPSA-3/TMSA)
36. Fractional Atomic Charge Weighted Partial Negative Surface Area (PNSA-3/TMSA)
37. Weighted Atomic Charge Weighted Partial Positive Surface Area (PPSA3*TMSA/1000)
38. Weighted Atomic Charge Weighted Partial Negative Surface Area (PNSA3*TMSA/1000)
39. Relative Positive Charge (Most Positive Charge / Total Positive Charge)
40. Relative Positive Charged Surface Area (Most Positive Surface Area * RPCG)
41. Relative Negative Charge (Most Negative Charge / Total Negative Charge)
42. Relative Negative Charged Surface Area (Most Negative Surface Area * RNCG)
43. Min(N_H-Acceptor, N_H-Donor)
44. Count of H-Acceptor Sites
45. Count of H-Donor Sites
46. HA Dependent H-Donors Surface Area-1
47. HA Dependent H-Donors Surface Area-1/TMSA
48. HA Dependent H-Donors Surface Area-2
49. HA Dependent H-Donors Surface Area-2/TMSA
50. HA Dependent H-Donors Surface Area-2/Sqrt(TMSA)
51. HA Dependent H-Donors Charged Surface Area-1
52. HA Dependent H-Donors Charged Surface Area-1/TMSA
53. HA Dependent H-Donors Charged Surface Area-2
54. HA Dependent H-Donors Charged Surface Area-2/TMSA
55. HA Dependent H-Donors Charged Surface Area-2/Sqrt(TMSA)
56. H-Acceptors Surface Area-1
57. H-Acceptors Surface Area-1/TMSA
58. H-Acceptors Surface Area-2
59. H-Acceptors Surface Area-2/TMSA
60. H-Acceptors Surface Area-2/Sqrt(TMSA)
61. H-Acceptors Charged Surface Area-1
62. H-Acceptors Charged Surface Area-1/TMSA
63. H-Acceptors Charged Surface Area-2
64. H-Acceptors Charged Surface Area-2/TMSA
65. H-Acceptors Charged Surface Area-2/Sqrt(TMSA)

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Molecular Descriptors

Constitutional Descriptors

1. Number of Atoms
2. Relative Number of C Atoms
3. Relative Number of H Atoms
4. Relative Number of O Atoms
5. Relative Number of N Atoms
6. Relative Number of S Atoms
7. Number of Single Bonds
8. Relative Number of Single Bonds
9. Relative Number of Double Bonds
10. Relative Number of Triple Bonds
11. Number of Aromatic Bonds
12. Relative Number of Aromatic Bonds
13. Relative Number of Rings
14. Relative Number of Benzene Rings
15. Molecular Weight
16. Relative Molecular Weight
17. Gravitation Index (All Bonds)
18. Gravitation Index (All Pairs)
19. Cubic Root of Gravitation Index (All Bonds)
20. Cubic Root of Gravitation Index (All Pairs)
21. Average Molecular Weight
22. Sum of Atomic Van Der Waals Volumes (Scaled on Carbon Atom)
23. Sum of Atomic Sanderson Electronegativities (Scaled on Carbon Atom)
24. Sum of Atomic Polarizabilities (Scaled on Carbon Atom)
25. Sum of Kier-Hall Electrotopological States
26. Mean Atomic Van Der Waals Volume (Scaled on Carbon Atom)
27. Mean Atomic Sanderson Electronegativity (Scaled on Carbon Atom)
28. Mean Atomic Polarizability (Scaled on Carbon Atom)
29. Mean Electrotopological State
30. Number of Non-H Atoms
31. Number of Bonds
32. Number of Non-H Bonds
33. Number of Multiple Bonds
34. Sum of Conventional Bond Orders (H-Depleted)
35. Aromatic Ratio
36. Number of Rings
37. Number of Circuits
38. Number of Rotatable Bonds

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39. Rotatable Bond Fraction
40. Number of Double Bonds
41. Number of Triple Bonds
42. Number of Conjugated Bonds
43. Number of Hydrogen Atoms
44. Number of Carbon Atoms
45. Number of Nitrogen Atoms
46. Number of Oxygen Atoms
47. Number of Sulfur Atoms
48. Number of 3-Membered Rings
49. Number of 4-Membered Rings
50. Number of 5-Membered Rings
51. Number of 6-Membered Rings
52. Number of 7-Membered Rings
53. Number of 8-Membered Rings
54. Number of 9-Membered Rings
55. Number of 10-Membered Rings
56. Number of 11-Membered Rings
57. Number of 12-Membered Rings
58. Number of Benzene-Like Rings

Topological Descriptors

1. Kier Molecular Flexibility Index
2. Average Information Content (Order 0)
3. Average Information Content (Order 1)
4. Average Information Content (Order 2)
5. Information Content (Order 0)
6. Information Content (Order 1)
7. Information Content (Order 2)
8. Average Structural Information Content (Order 0)
9. Average Structural Information Content (Order 1)
10. Average Structural Information Content (Order 2)
11. Structural Information Content (Order 0)
12. Structural Information Content (Order 1)
13. Structural Information Content (Order 2)
14. Average Complementary Information Content (Order 0)
15. Average Complementary Information Content (Order 1)
16. Average Complementary Information Content (Order 2)
17. Complementary Information Content (Order 0)
18. Complementary Information Content (Order 1)
19. Complementary Information Content (Order 2)
20. Average Bonding Information Content (Order 0)
21. Average Bonding Information Content (Order 1)
22. Average Bonding Information Content (Order 2)
23. Bonding Information Content (Order 0)

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24. Bonding Information Content (Order 1)
25. Bonding Information Content (Order 2)
26. Balaban Index
27. First Zagreb Index M1
28. First Zagreb Index by Valence Vertex Degrees
29. Second Zagreb Index M2
30. Second Zagreb Index by Valence Vertex Degrees
31. Quadratic Index
32. Narumi Simple Topological Index (Log S)
33. Narumi Harmonic Topological Index (H)
34. Narumi Geometric Topological Index (G)
35. Total Structure Connectivity Index
36. Pogliani Index
37. Ramification Index
38. Polarity Number
39. Log of Product of Row Sums (PRS Index)
40. Average Vertex Distance Degree
41. Mean Square Distance Index (Balaban)
42. Schultz Molecular Topological Index
43. Schultz Molecular Topological Index by Valence Vertex Degrees
44. Gutman Molecular Topological Index
45. Gutman Molecular Topological Index by Valence Vertex Degrees
46. Xu Index
47. Superpendentic Index
48. Wiener W Index
49. Mean Wiener Index
50. Harary H Index
51. Square Reciprocal Distance Sum Index
52. Quasi-Wiener Index
53. First Mohar Index TI1
54. Second Mohar Index TI2
55. Spanning Tree Number (Log)
56. Hyper-Distance-Path Index
57. Reciprocal Hyper-Distance-Path Index
58. Detour Index
59. Hyper-Detour Index
60. Reciprocal Hyper-Detour Index
61. Distance/Detour Index
62. All-Path Wiener Index
63. Wiener-Type Index (Barysz Distance Matrix)
64. Wiener-Type Index (Mass Weighted Distance Matrix)
65. Wiener-Type Index (Van Der Waals Weighted Distantce Matrix)
66. Wiener-Type Index (Electronegativity Weighted Distance Matrix)
67. Wiener-Type Index (Polarizability Weighted Distance Matrix)
68. Balaban Distance Connectivity Index
69. Balaban-Type Index (Barysz Distance Matrix)

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70. Balaban-Type Index (Mass Weighted Distance Matrix)
71. Balaban-Type Index (Van Der Waals Weighted Distantce Matrix)
72. Balaban-Type Index (Electronegativity Weighted Distance Matrix)
73. Balaban-Type Index (Polarizability Weighted Distance Matrix)
74. Maximal Electrotopological Negative Variation
75. Maximal Electrotopological Positive Variation
76. Molecular Electrotopological Variation
77. Elctrotopological State Topological Parameter
78. Kier Symmetry Index
79. Kier Alpha-Modified Shape Index M1
80. Kier Alpha-Modified Shape Index M2
81. Kier Alpha-Modified Shape Index M3
82. Kier Benzene-Likeliness Index
83. Path/Walk Shape Index M2
84. Path/Walk Shape Index M3
85. Path/Walk Shape Index M4
86. Path/Walk Shape Index M5
87. 2D Petitjean Shape Index
88. Eccentric Connectivity Index
89. Eccentricity
90. Average Eccentricity
91. Eccentric
92. Mean Distance Degree Deviation
93. Unipolarity
94. Centralization
95. Variation
96. Balaban Centric Index
97. Lopping Centric Information Index
98. Radial Centric Information Index
99. Distance/Detour Ring Index (Order 3)
100. Distance/Detour Ring Index (Order 4)
101. Distance/Detour Ring Index (Order 5)
102. Distance/Detour Ring Index (Order 6)
103. Distance/Detour Ring Index (Order 7)
104. Distance/Detour Ring Index (Order 8)
105. Distance/Detour Ring Index (Order 9)
106. Distance/Detour Ring Index (Order 10)
107. Distance/Detour Ring Index (Order 11)
108. Distance/Detour Ring Index (Order 12)
109. Sum of Topological Distances Between N..N
110. Sum of Topological Distances Between N..O
111. Sum of Topological Distances Between N..S
112. Sum of Topological Distances Between O..O
113. Sum of Topological Distances Between O..S
114. Sum of Topological Distances Between S..S

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Walk And Path Counts

1. Molecular Walk Count K1
2. Molecular Walk Count K2
3. Molecular Walk Count K3
4. Molecular Walk Count K4
5. Molecular Walk Count K5
6. Molecular Walk Count K6
7. Molecular Walk Count K7
8. Molecular Walk Count K8
9. Molecular Walk Count K9
10. Molecular Walk Count K10
11. Total Walk Count
12. Self-Returning Walk Count K1
13. Self-Returning Walk Count K2
14. Self-Returning Walk Count K3
15. Self-Returning Walk Count K4
16. Self-Returning Walk Count K5
17. Self-Returning Walk Count K6
18. Self-Returning Walk Count K7
19. Self-Returning Walk Count K8
20. Self-Returning Walk Count K9
21. Self-Returning Walk Count K10
22. Molecular Path Count M1
23. Molecular Path Count M2
24. Molecular Path Count M3
25. Molecular Path Count M4
26. Molecular Path Count M5
27. Molecular Path Count M6
28. Molecular Path Count M7
29. Molecular Path Count M8
30. Molecular Path Count M9
31. Molecular Path Count M10
32. Molecular Multiple Path Count M1
33. Molecular Multiple Path Count M2
34. Molecular Multiple Path Count M3
35. Molecular Multiple Path Count M4
36. Molecular Multiple Path Count M5
37. Molecular Multiple Path Count M6
38. Molecular Multiple Path Count M7
39. Molecular Multiple Path Count M8
40. Molecular Multiple Path Count M9
41. Molecular Multiple Path Count M10
42. Total Path Count
43. Conventional Bond-Order ID Number
44. Ratio of Multiple Path Count Over Path Count

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45. Difference Between Multiple Path Count and Path Count
46. Randic Connectivity ID Number
47. Balaban ID Number

Connectivity Indices

1. Connectivity Index M0
2. Connectivity Index M1
3. Connectivity Index M2
4. Connectivity Index M3
5. Connectivity Index M4
6. Connectivity Index M5
7. Average Connectivity Index M0
8. Average Connectivity Index M1
9. Average Connectivity Index M2
10. Average Connectivity Index M3
11. Average Connectivity Index M4
12. Average Connectivity Index M5
13. Valence Connectivity Index M0
14. Valence Connectivity Index M1
15. Valence Connectivity Index M2
16. Valence Connectivity Index M3
17. Valence Connectivity Index M4
18. Valence Connectivity Index M5
19. Average Valence Connectivity Index M0
20. Average Valence Connectivity Index M1
21. Average Valence Connectivity Index M2
22. Average Valence Connectivity Index M3
23. Average Valence Connectivity Index M4
24. Average Valence Connectivity Index M5
25. Solvation Connectivity Index M0
26. Solvation Connectivity Index M1
27. Solvation Connectivity Index M2
28. Solvation Connectivity Index M3
29. Solvation Connectivity Index M4
30. Solvation Connectivity Index M5
31. Modified Randic Connectivity Index
32. Reciprocal Distance Randic-Type Index
33. Reciprocal Distance Squared Randic-Type Index

Information Indices

1. Information Index on Molecular Size
2. Total Information Index of Atomic Composition
3. Mean Information Index on Atomic Composition
4. Mean Information Content on the Distance Equality

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5. Mean Information Content on the Distance Magnitude
6. Mean Information Content on the Distance Degree Equality
7. Mean Information Content on the Distance Degree Magnitude
8. Total Information Content on the Distance Equality
9. Total Information Content on the Distance Magnitude
10. Mean Information Content on the Vertex Degree Equality
11. Mean Information Content on the Vertex Degree Magnitude
12. Graph Vertex Complexity Index
13. Graph Distance Complexity Index (Log)
14. Balaban U Index
15. Balaban V Index
16. Balaban X Index
17. Balaban Y Index
18. Information Content Index Level0
19. Total Information Content Index Level0
20. Structural Information Content Level0
21. Complementary Information Content Level0
22. Bond Information Content Level0
23. Information Content Index Level1
24. Total Information Content Index Level1
25. Structural Information Content Level1
26. Complementary Information Content Level1
27. Bond Information Content Level1
28. Information Content Index Level2
29. Total Information Content Index Level2
30. Structural Information Content Level2
31. Complementary Information Content Level2
32. Bond Information Content Level2
33. Information Content Index Level3
34. Total Information Content Index Level3
35. Structural Information Content Level3
36. Complementary Information Content Level3
37. Bond Information Content Level3
38. Information Content Index Level4
39. Total Information Content Index Level4
40. Structural Information Content Level4
41. Complementary Information Content Level4
42. Bond Information Content Level4
43. Information Content Index Level5
44. Total Information Content Index Level5
45. Structural Information Content Level5
46. Complementary Information Content Level5
47. Bond Information Content Level5

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2D Autocorrelation Indices

1. Broto-Moreau Autocorrelation D1 (Atomic Masses)
2. Broto-Moreau Autocorrelation D2 (Atomic Masses)
3. Broto-Moreau Autocorrelation D3 (Atomic Masses)
4. Broto-Moreau Autocorrelation D4 (Atomic Masses)
5. Broto-Moreau Autocorrelation D5 (Atomic Masses)
6. Broto-Moreau Autocorrelation D6 (Atomic Masses)
7. Broto-Moreau Autocorrelation D7 (Atomic Masses)
8. Broto-Moreau Autocorrelation D8 (Atomic Masses)
9. Broto-Moreau Autocorrelation D1 (Atomic van der Waals Volumes)
10. Broto-Moreau Autocorrelation D2 (Atomic van der Waals Volumes)
11. Broto-Moreau Autocorrelation D3 (Atomic van der Waals Volumes)
12. Broto-Moreau Autocorrelation D4 (Atomic van der Waals Volumes)
13. Broto-Moreau Autocorrelation D5 (Atomic van der Waals Volumes)
14. Broto-Moreau Autocorrelation D6 (Atomic van der Waals Volumes)
15. Broto-Moreau Autocorrelation D7 (Atomic van der Waals Volumes)
16. Broto-Moreau Autocorrelation D8 (Atomic van der Waals Volumes)
17. Broto-Moreau Autocorrelation D1 (Atomic Sanderson Electronegativities)
18. Broto-Moreau Autocorrelation D2 (Atomic Sanderson Electronegativities)
19. Broto-Moreau Autocorrelation D3 (Atomic Sanderson Electronegativities)
20. Broto-Moreau Autocorrelation D4 (Atomic Sanderson Electronegativities)
21. Broto-Moreau Autocorrelation D5 (Atomic Sanderson Electronegativities)
22. Broto-Moreau Autocorrelation D6 (Atomic Sanderson Electronegativities)
23. Broto-Moreau Autocorrelation D7 (Atomic Sanderson Electronegativities)
24. Broto-Moreau Autocorrelation D8 (Atomic Sanderson Electronegativities)
25. Broto-Moreau Autocorrelation D1 (Atomic Polarizabilities)
26. Broto-Moreau Autocorrelation D2 (Atomic Polarizabilities)
27. Broto-Moreau Autocorrelation D3 (Atomic Polarizabilities)
28. Broto-Moreau Autocorrelation D4 (Atomic Polarizabilities)
29. Broto-Moreau Autocorrelation D5 (Atomic Polarizabilities)
30. Broto-Moreau Autocorrelation D6 (Atomic Polarizabilities)
31. Broto-Moreau Autocorrelation D7 (Atomic Polarizabilities)
32. Broto-Moreau Autocorrelation D8 (Atomic Polarizabilities)
33. Moran Autocorrelation D1 (Atomic Masses)
34. Moran Autocorrelation D2 (Atomic Masses)
35. Moran Autocorrelation D3 (Atomic Masses)
36. Moran Autocorrelation D4 (Atomic Masses)
37. Moran Autocorrelation D5 (Atomic Masses)
38. Moran Autocorrelation D6 (Atomic Masses)
39. Moran Autocorrelation D7 (Atomic Masses)
40. Moran Autocorrelation D8 (Atomic Masses)
41. Moran Autocorrelation D1 (Atomic van der Waals Volumes)
42. Moran Autocorrelation D2 (Atomic van der Waals Volumes)
43. Moran Autocorrelation D3 (Atomic van der Waals Volumes)
44. Moran Autocorrelation D4 (Atomic van der Waals Volumes)

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45. Moran Autocorrelation D5 (Atomic van der Waals Volumes)
46. Moran Autocorrelation D6 (Atomic van der Waals Volumes)
47. Moran Autocorrelation D7 (Atomic van der Waals Volumes)
48. Moran Autocorrelation D8 (Atomic van der Waals Volumes)
49. Moran Autocorrelation D1 (Atomic Sanderson Electronegativities)
50. Moran Autocorrelation D2 (Atomic Sanderson Electronegativities)
51. Moran Autocorrelation D3 (Atomic Sanderson Electronegativities)
52. Moran Autocorrelation D4 (Atomic Sanderson Electronegativities)
53. Moran Autocorrelation D5 (Atomic Sanderson Electronegativities)
54. Moran Autocorrelation D6 (Atomic Sanderson Electronegativities)
55. Moran Autocorrelation D7 (Atomic Sanderson Electronegativities)
56. Moran Autocorrelation D8 (Atomic Sanderson Electronegativities)
57. Moran Autocorrelation D1 (Atomic Polarizabilities)
58. Moran Autocorrelation D2 (Atomic Polarizabilities)
59. Moran Autocorrelation D3 (Atomic Polarizabilities)
60. Moran Autocorrelation D4 (Atomic Polarizabilities)
61. Moran Autocorrelation D5 (Atomic Polarizabilities)
62. Moran Autocorrelation D6 (Atomic Polarizabilities)
63. Moran Autocorrelation D7 (Atomic Polarizabilities)
64. Moran Autocorrelation D8 (Atomic Polarizabilities)
65. Geary Autocorrelation D1 (Atomic Masses)
66. Geary Autocorrelation D2 (Atomic Masses)
67. Geary Autocorrelation D3 (Atomic Masses)
68. Geary Autocorrelation D4 (Atomic Masses)
69. Geary Autocorrelation D5 (Atomic Masses)
70. Geary Autocorrelation D6 (Atomic Masses)
71. Geary Autocorrelation D7 (Atomic Masses)
72. Geary Autocorrelation D8 (Atomic Masses)
73. Geary Autocorrelation D1 (Atomic van der Waals Volumes)
74. Geary Autocorrelation D2 (Atomic van der Waals Volumes)
75. Geary Autocorrelation D3 (Atomic van der Waals Volumes)
76. Geary Autocorrelation D4 (Atomic van der Waals Volumes)
77. Geary Autocorrelation D5 (Atomic van der Waals Volumes)
78. Geary Autocorrelation D6 (Atomic van der Waals Volumes)
79. Geary Autocorrelation D7 (Atomic van der Waals Volumes)
80. Geary Autocorrelation D8 (Atomic van der Waals Volumes)
81. Geary Autocorrelation D1 (Atomic Sanderson Electronegativities)
82. Geary Autocorrelation D2 (Atomic Sanderson Electronegativities)
83. Geary Autocorrelation D3 (Atomic Sanderson Electronegativities)
84. Geary Autocorrelation D4 (Atomic Sanderson Electronegativities)
85. Geary Autocorrelation D5 (Atomic Sanderson Electronegativities)
86. Geary Autocorrelation D6 (Atomic Sanderson Electronegativities)
87. Geary Autocorrelation D7 (Atomic Sanderson Electronegativities)
88. Geary Autocorrelation D8 (Atomic Sanderson Electronegativities)
89. Geary Autocorrelation D1 (Atomic Polarizabilities)
90. Geary Autocorrelation D2 (Atomic Polarizabilities)

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91. Geary Autocorrelation D3 (Atomic Polarizabilities)
92. Geary Autocorrelation D4 (Atomic Polarizabilities)
93. Geary Autocorrelation D5 (Atomic Polarizabilities)
94. Geary Autocorrelation D6 (Atomic Polarizabilities)
95. Geary Autocorrelation D7 (Atomic Polarizabilities)
96. Geary Autocorrelation D8 (Atomic Polarizabilities)

Edge Adjacency Indices

1. Edge Connectivity Index (Order 0)
2. Edge Connectivity Index (Order 1)
3. Eigenvalue 1 of Edge Adjacency Matrix (Edge Degrees)
4. Eigenvalue 2 of Edge Adjacency Matrix (Edge Degrees)
5. Eigenvalue 3 of Edge Adjacency Matrix (Edge Degrees)
6. Eigenvalue 4 of Edge Adjacency Matrix (Edge Degrees)
7. Eigenvalue 5 of Edge Adjacency Matrix (Edge Degrees)
8. Eigenvalue 6 of Edge Adjacency Matrix (Edge Degrees)
9. Eigenvalue 7 of Edge Adjacency Matrix (Edge Degrees)
10. Eigenvalue 8 of Edge Adjacency Matrix (Edge Degrees)
11. Eigenvalue 9 of Edge Adjacency Matrix (Edge Degrees)
12. Eigenvalue 10 of Edge Adjacency Matrix (Edge Degrees)
13. Eigenvalue 11 of Edge Adjacency Matrix (Edge Degrees)
14. Eigenvalue 12 of Edge Adjacency Matrix (Edge Degrees)
15. Eigenvalue 13 of Edge Adjacency Matrix (Edge Degrees)
16. Eigenvalue 14 of Edge Adjacency Matrix (Edge Degrees)
17. Eigenvalue 15 of Edge Adjacency Matrix (Edge Degrees)
18. Eigenvalue 1 of Edge Adjacency Matrix (Dipole Moments)
19. Eigenvalue 2 of Edge Adjacency Matrix (Dipole Moments)
20. Eigenvalue 3 of Edge Adjacency Matrix (Dipole Moments)
21. Eigenvalue 4 of Edge Adjacency Matrix (Dipole Moments)
22. Eigenvalue 5 of Edge Adjacency Matrix (Dipole Moments)
23. Eigenvalue 6 of Edge Adjacency Matrix (Dipole Moments)
24. Eigenvalue 7 of Edge Adjacency Matrix (Dipole Moments)
25. Eigenvalue 8 of Edge Adjacency Matrix (Dipole Moments)
26. Eigenvalue 9 of Edge Adjacency Matrix (Dipole Moments)
27. Eigenvalue 10 of Edge Adjacency Matrix (Dipole Moments)
28. Eigenvalue 11 of Edge Adjacency Matrix (Dipole Moments)
29. Eigenvalue 12 of Edge Adjacency Matrix (Dipole Moments)
30. Eigenvalue 13 of Edge Adjacency Matrix (Dipole Moments)
31. Eigenvalue 14 of Edge Adjacency Matrix (Dipole Moments)
32. Eigenvalue 15 of Edge Adjacency Matrix (Dipole Moments)
33. Eigenvalue 1 of Edge Adjacency Matrix (Resonance Integrals)
34. Eigenvalue 2 of Edge Adjacency Matrix (Resonance Integrals)
35. Eigenvalue 3 of Edge Adjacency Matrix (Resonance Integrals)
36. Eigenvalue 4 of Edge Adjacency Matrix (Resonance Integrals)
37. Eigenvalue 5 of Edge Adjacency Matrix (Resonance Integrals)

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38. Eigenvalue 6 of Edge Adjacency Matrix (Resonance Integrals)
39. Eigenvalue 7 of Edge Adjacency Matrix (Resonance Integrals)
40. Eigenvalue 8 of Edge Adjacency Matrix (Resonance Integrals)
41. Eigenvalue 9 of Edge Adjacency Matrix (Resonance Integrals)
42. Eigenvalue 10 of Edge Adjacency Matrix (Resonance Integrals)
43. Eigenvalue 11 of Edge Adjacency Matrix (Resonance Integrals)
44. Eigenvalue 12 of Edge Adjacency Matrix (Resonance Integrals)
45. Eigenvalue 13 of Edge Adjacency Matrix (Resonance Integrals)
46. Eigenvalue 14 of Edge Adjacency Matrix (Resonance Integrals)
47. Eigenvalue 15 of Edge Adjacency Matrix (Resonance Integrals)
48. Spectral Moment 1 of Edge Adjacency Matrix
49. Spectral Moment 2 of Edge Adjacency Matrix
50. Spectral Moment 3 of Edge Adjacency Matrix
51. Spectral Moment 4 of Edge Adjacency Matrix
52. Spectral Moment 5 of Edge Adjacency Matrix
53. Spectral Moment 6 of Edge Adjacency Matrix
54. Spectral Moment 7 of Edge Adjacency Matrix
55. Spectral Moment 8 of Edge Adjacency Matrix
56. Spectral Moment 9 of Edge Adjacency Matrix
57. Spectral Moment 10 of Edge Adjacency Matrix
58. Spectral Moment 11 of Edge Adjacency Matrix
59. Spectral Moment 12 of Edge Adjacency Matrix
60. Spectral Moment 13 of Edge Adjacency Matrix
61. Spectral Moment 14 of Edge Adjacency Matrix
62. Spectral Moment 15 of Edge Adjacency Matrix
63. Spectral Moment 1 of Edge Adjacency Matrix (Edge Degrees)
64. Spectral Moment 2 of Edge Adjacency Matrix (Edge Degrees)
65. Spectral Moment 3 of Edge Adjacency Matrix (Edge Degrees)
66. Spectral Moment 4 of Edge Adjacency Matrix (Edge Degrees)
67. Spectral Moment 5 of Edge Adjacency Matrix (Edge Degrees)
68. Spectral Moment 6 of Edge Adjacency Matrix (Edge Degrees)
69. Spectral Moment 7 of Edge Adjacency Matrix (Edge Degrees)
70. Spectral Moment 8 of Edge Adjacency Matrix (Edge Degrees)
71. Spectral Moment 9 of Edge Adjacency Matrix (Edge Degrees)
72. Spectral Moment 10 of Edge Adjacency Matrix (Edge Degrees)
73. Spectral Moment 11 of Edge Adjacency Matrix (Edge Degrees)
74. Spectral Moment 12 of Edge Adjacency Matrix (Edge Degrees)
75. Spectral Moment 13 of Edge Adjacency Matrix (Edge Degrees)
76. Spectral Moment 14 of Edge Adjacency Matrix (Edge Degrees)
77. Spectral Moment 15 of Edge Adjacency Matrix (Edge Degrees)
78. Spectral Moment 1 of Edge Adjacency Matrix (Dipole Moments)
79. Spectral Moment 2 of Edge Adjacency Matrix (Dipole Moments)
80. Spectral Moment 3 of Edge Adjacency Matrix (Dipole Moments)
81. Spectral Moment 4 of Edge Adjacency Matrix (Dipole Moments)
82. Spectral Moment 5 of Edge Adjacency Matrix (Dipole Moments)
83. Spectral Moment 6 of Edge Adjacency Matrix (Dipole Moments)

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84. Spectral Moment 7 of Edge Adjacency Matrix (Dipole Moments)
85. Spectral Moment 8 of Edge Adjacency Matrix (Dipole Moments)
86. Spectral Moment 9 of Edge Adjacency Matrix (Dipole Moments)
87. Spectral Moment 10 of Edge Adjacency Matrix (Dipole Moments)
88. Spectral Moment 11 of Edge Adjacency Matrix (Dipole Moments)
89. Spectral Moment 12 of Edge Adjacency Matrix (Dipole Moments)
90. Spectral Moment 13 of Edge Adjacency Matrix (Dipole Moments)
91. Spectral Moment 14 of Edge Adjacency Matrix (Dipole Moments)
92. Spectral Moment 15 of Edge Adjacency Matrix (Dipole Moments)
93. Spectral Moment 1 of Edge Adjacency Matrix (Resonance Integrals)
94. Spectral Moment 2 of Edge Adjacency Matrix (Resonance Integrals)
95. Spectral Moment 3 of Edge Adjacency Matrix (Resonance Integrals)
96. Spectral Moment 4 of Edge Adjacency Matrix (Resonance Integrals)
97. Spectral Moment 5 of Edge Adjacency Matrix (Resonance Integrals)
98. Spectral Moment 6 of Edge Adjacency Matrix (Resonance Integrals)
99. Spectral Moment 7 of Edge Adjacency Matrix (Resonance Integrals)
100. Spectral Moment 8 of Edge Adjacency Matrix (Resonance Integrals)
101. Spectral Moment 9 of Edge Adjacency Matrix (Resonance Integrals)
102. Spectral Moment 10 of Edge Adjacency Matrix (Resonance Integrals)
103. Spectral Moment 11 of Edge Adjacency Matrix (Resonance Integrals)
104. Spectral Moment 12 of Edge Adjacency Matrix (Resonance Integrals)
105. Spectral Moment 13 of Edge Adjacency Matrix (Resonance Integrals)
106. Spectral Moment 14 of Edge Adjacency Matrix (Resonance Integrals)
107. Spectral Moment 15 of Edge Adjacency Matrix (Resonance Integrals)

Burden Eigenvalue Descriptors

1. Highest Positive Eigenvalue K1 of Burden Matrix (Atomic Masses)
2. Highest Positive Eigenvalue K2 of Burden Matrix (Atomic Masses)
3. Highest Positive Eigenvalue K3 of Burden Matrix (Atomic Masses)
4. Highest Positive Eigenvalue K4 of Burden Matrix (Atomic Masses)
5. Highest Positive Eigenvalue K5 of Burden Matrix (Atomic Masses)
6. Highest Positive Eigenvalue K6 of Burden Matrix (Atomic Masses)
7. Highest Positive Eigenvalue K7 of Burden Matrix (Atomic Masses)
8. Highest Positive Eigenvalue K8 of Burden Matrix (Atomic Masses)
9. Lowest Negative Eigenvalue K1 of Burden Matrix (Atomic Masses)
10. Lowest Negative Eigenvalue K2 of Burden Matrix (Atomic Masses)
11. Lowest Negative Eigenvalue K3 of Burden Matrix (Atomic Masses)
12. Lowest Negative Eigenvalue K4 of Burden Matrix (Atomic Masses)
13. Lowest Negative Eigenvalue K5 of Burden Matrix (Atomic Masses)
14. Lowest Negative Eigenvalue K6 of Burden Matrix (Atomic Masses)
15. Lowest Negative Eigenvalue K7 of Burden Matrix (Atomic Masses)
16. Lowest Negative Eigenvalue K8 of Burden Matrix (Atomic Masses)
17. Highest Positive Eigenvalue K1 of Burden Matrix (Atomic van der Waals Volumes)
18. Highest Positive Eigenvalue K2 of Burden Matrix (Atomic van der Waals Volumes)
19. Highest Positive Eigenvalue K3 of Burden Matrix (Atomic van der Waals Volumes)

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20. Highest Positive Eigenvalue K4 of Burden Matrix (Atomic van der Waals Volumes)
21. Highest Positive Eigenvalue K5 of Burden Matrix (Atomic van der Waals Volumes)
22. Highest Positive Eigenvalue K6 of Burden Matrix (Atomic van der Waals Volumes)
23. Highest Positive Eigenvalue K7 of Burden Matrix (Atomic van der Waals Volumes)
24. Highest Positive Eigenvalue K8 of Burden Matrix (Atomic van der Waals Volumes)
25. Lowest Negative Eigenvalue K1 of Burden Matrix (Atomic van der Waals Volumes)
26. Lowest Negative Eigenvalue K2 of Burden Matrix (Atomic van der Waals Volumes)
27. Lowest Negative Eigenvalue K3 of Burden Matrix (Atomic van der Waals Volumes)
28. Lowest Negative Eigenvalue K4 of Burden Matrix (Atomic van der Waals Volumes)
29. Lowest Negative Eigenvalue K5 of Burden Matrix (Atomic van der Waals Volumes)
30. Lowest Negative Eigenvalue K6 of Burden Matrix (Atomic van der Waals Volumes)
31. Lowest Negative Eigenvalue K7 of Burden Matrix (Atomic van der Waals Volumes)
32. Lowest Negative Eigenvalue K8 of Burden Matrix (Atomic van der Waals Volumes)
33. Highest Positive Eigenvalue K1 of Burden Matrix (Atomic Sanderson Electronegativities)
34. Highest Positive Eigenvalue K2 of Burden Matrix (Atomic Sanderson Electronegativities)
35. Highest Positive Eigenvalue K3 of Burden Matrix (Atomic Sanderson Electronegativities)
36. Highest Positive Eigenvalue K4 of Burden Matrix (Atomic Sanderson Electronegativities)
37. Highest Positive Eigenvalue K5 of Burden Matrix (Atomic Sanderson Electronegativities)
38. Highest Positive Eigenvalue K6 of Burden Matrix (Atomic Sanderson Electronegativities)
39. Highest Positive Eigenvalue K7 of Burden Matrix (Atomic Sanderson Electronegativities)
40. Highest Positive Eigenvalue K8 of Burden Matrix (Atomic Sanderson Electronegativities)
41. Lowest Negative Eigenvalue K1 of Burden Matrix (Atomic Sanderson Electronegativities)
42. Lowest Negative Eigenvalue K2 of Burden Matrix (Atomic Sanderson Electronegativities)
43. Lowest Negative Eigenvalue K3 of Burden Matrix (Atomic Sanderson Electronegativities)
44. Lowest Negative Eigenvalue K4 of Burden Matrix (Atomic Sanderson Electronegativities)
45. Lowest Negative Eigenvalue K5 of Burden Matrix (Atomic Sanderson Electronegativities)
46. Lowest Negative Eigenvalue K6 of Burden Matrix (Atomic Sanderson Electronegativities)
47. Lowest Negative Eigenvalue K7 of Burden Matrix (Atomic Sanderson Electronegativities)
48. Lowest Negative Eigenvalue K8 of Burden Matrix (Atomic Sanderson Electronegativities)
49. Highest Positive Eigenvalue K1 of Burden Matrix (Atomic Polarizabilities)
50. Highest Positive Eigenvalue K2 of Burden Matrix (Atomic Polarizabilities)
51. Highest Positive Eigenvalue K3 of Burden Matrix (Atomic Polarizabilities)
52. Highest Positive Eigenvalue K4 of Burden Matrix (Atomic Polarizabilities)
53. Highest Positive Eigenvalue K5 of Burden Matrix (Atomic Polarizabilities)
54. Highest Positive Eigenvalue K6 of Burden Matrix (Atomic Polarizabilities)
55. Highest Positive Eigenvalue K7 of Burden Matrix (Atomic Polarizabilities)
56. Highest Positive Eigenvalue K8 of Burden Matrix (Atomic Polarizabilities)
57. Lowest Negative Eigenvalue K1 of Burden Matrix (Atomic Polarizabilities)
58. Lowest Negative Eigenvalue K2 of Burden Matrix (Atomic Polarizabilities)
59. Lowest Negative Eigenvalue K3 of Burden Matrix (Atomic Polarizabilities)
60. Lowest Negative Eigenvalue K4 of Burden Matrix (Atomic Polarizabilities)
61. Lowest Negative Eigenvalue K5 of Burden Matrix (Atomic Polarizabilities)
62. Lowest Negative Eigenvalue K6 of Burden Matrix (Atomic Polarizabilities)
63. Lowest Negative Eigenvalue K7 of Burden Matrix (Atomic Polarizabilities)
64. Lowest Negative Eigenvalue K8 of Burden Matrix (Atomic Polarizabilities)

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Topological Charge Indices

1. Topological Charge Index K1
2. Topological Charge Index K2
3. Topological Charge Index K3
4. Topological Charge Index K4
5. Topological Charge Index K5
6. Topological Charge Index K6
7. Topological Charge Index K7
8. Topological Charge Index K8
9. Topological Charge Index K9
10. Topological Charge Index K10
11. Mean Topological Charge Index K1
12. Mean Topological Charge Index K2
13. Mean Topological Charge Index K3
14. Mean Topological Charge Index K4
15. Mean Topological Charge Index K5
16. Mean Topological Charge Index K6
17. Mean Topological Charge Index K7
18. Mean Topological Charge Index K8
19. Mean Topological Charge Index K9
20. Mean Topological Charge Index K10
21. Global Topological Charge Index

Eigenvalue-Based Indices

1. Lovasz-Pelikan Index (Leading Eigenvalue)
2. Leading Eigenvalue (Barysz Distance Matrix)
3. Leading Eigenvalue (Mass Weighted Distance Matrix)
4. Leading Eigenvalue (van der Waals Weighted Distance Matrix)
5. Leading Eigenvalue (Electronegativity Weighted Distance Matrix)
6. Leading Eigenvalue (Polarizability Weighted Distance Matrix)
7. Eigenvalue Sum (Barysz Distance Matrix)
8. Eigenvalue Sum (Mass Weighted Distance Matrix)
9. Eigenvalue Sum (van der Waals Weighted Distance Matrix)
10. Eigenvalue Sum (Electronegativity Weighted Distance Matrix)
11. Eigenvalue Sum (Polarizability Weighted Distance Matrix)
12. Abs. Eigenvalue Sum (Barysz Distance Matrix)
13. Abs. Eigenvalue Sum (Mass Weighted Distance Matrix)
14. Abs. Eigenvalue Sum (van der Waals Weighted Distance Matrix)
15. Abs. Eigenvalue Sum (Electronegativity Weighted Distance Matrix)
16. Abs. Eigenvalue Sum (Polarizability Weighted Distance Matrix)
17. Eigenvector Coeff. Sum (Adjacency Matrix)
18. Avg Eigenvector Coeff. Sum (Adjacency Matrix)
19. Randic-Type Eigenvector Coeff. Sum (Adjacency Matrix)
20. Avg Randic-Type Eigenvector-Based Index (Adjacency Matrix)

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21. Eigenvector Coeff. Sum (Distance Matrix)
22. Avg Eigenvector Coeff. Sum (Distance Matrix)
23. Randic-Type Eigenvector Coeff. Sum (Distance Matrix)
24. Avg Randic-Type Eigenvector-Based Index (Distance Matrix)
25. Eigenvector Coeff. Sum (Barysz Distance Matrix)
26. Avg Eigenvector Coeff. Sum (Barysz Distance Matrix)
27. Randic-Type Eigenvector Coeff. Sum (Barysz Distance Matrix)
28. Avg Randic-Type Eigenvector-Based Index (Barysz Distance Matrix)
29. Eigenvector Coeff. Sum (Mass Weighted Distance Matrix)
30. Avg Eigenvector Coeff. Sum (Mass Weighted Distance Matrix)
31. Randic-Type Eigenvector Coeff. Sum (Mass Weighted Distance Matrix)
32. Avg Randic-Type Eigenvector-Based Index (Mass Weighted Distance Matrix)
33. Eigenvector Coeff. Sum (van der Waals Weighted Distance Matrix)
34. Avg Eigenvector Coeff. Sum (van der Waals Weighted Distance Matrix)
35. Randic-Type Eigenvector Coeff. Sum (van der Waals Weighted Distance Matrix)
36. Avg Randic-Type Eigenvector-Based Index (van der Waals Weighted Distance Matrix)
37. Eigenvector Coeff. Sum (Electronegativity Weighted Distance Matrix)
38. Avg Eigenvector Coeff. Sum (Electronegativity Weighted Distance Matrix)
39. Randic-Type Eigenvector Coeff. Sum (Electronegativity Weighted Distance Matrix)
40. Avg Randic-Type Eigenvector-Based Index (Electronegativity Weighted Distance Matrix)
41. Eigenvector Coeff. Sum (Polarizability Weighted Distance Matrix)
42. Avg Eigenvector Coeff. Sum (Polarizability Weighted Distance Matrix)
43. Randic-Type Eigenvector Coeff. Sum (Polarizability Weighted Distance Matrix)
44. Avg Randic-Type Eigenvector-Based Index (Polarizability Weighted Distance Matrix)

Randic Molecular Profiles

1. Randic Molecular Profile K1
2. Randic Molecular Profile K2
3. Randic Molecular Profile K3
4. Randic Molecular Profile K4
5. Randic Molecular Profile K5
6. Randic Molecular Profile K6
7. Randic Molecular Profile K7
8. Randic Molecular Profile K8
9. Randic Molecular Profile K9
10. Randic Molecular Profile K10
11. Randic Molecular Profile K11
12. Randic Molecular Profile K12
13. Randic Molecular Profile K13
14. Randic Molecular Profile K14
15. Randic Molecular Profile K15
16. Randic Molecular Profile K16
17. Randic Molecular Profile K17
18. Randic Molecular Profile K18
19. Randic Molecular Profile K19

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20. Randic Molecular Profile K20
21. Randic Shape Profile K1
22. Randic Shape Profile K2
23. Randic Shape Profile K3
24. Randic Shape Profile K4
25. Randic Shape Profile K5
26. Randic Shape Profile K6
27. Randic Shape Profile K7
28. Randic Shape Profile K8
29. Randic Shape Profile K9
30. Randic Shape Profile K10
31. Randic Shape Profile K11
32. Randic Shape Profile K12
33. Randic Shape Profile K13
34. Randic Shape Profile K14
35. Randic Shape Profile K15
36. Randic Shape Profile K16
37. Randic Shape Profile K17
38. Randic Shape Profile K18
39. Randic Shape Profile K19
40. Randic Shape Profile K20
41. Average Randic Shape Profile Index (Order 2)

Geometrical Descriptors

1. Moment of Inertia A
2. Moment of Inertia B
3. Moment of Inertia C
4. XY Shadow
5. XY Shadow / XY Rectangle
6. YZ Shadow
7. YZ Shadow / YZ Rectangle
8. ZX Shadow
9. ZX Shadow / ZX Rectangle
10. Molecular Volume
11. Molecular Volume / XYZ Box
12. Molecular Surface Area
13. 3D-Wiener Index
14. 3D-Balaban Index
15. 3D-Harary Index
16. Average Geometric Distance Degree
17. Distance/Distance Index
18. Average Distance/Distance Degree
19. Gravitational Index G1
20. Gravitational Index G2 (Bond-Restricted)
21. Radius of Gyration (Mass Weighted)

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22. Span R
23. Average Span R
24. Molecular Eccentricity
25. Spherosity Index
26. Asphericity Index
27. Folding Degree Index
28. 3D Petitjean Shape Index
29. Length / Breadth by Whim
30. Absolute Eigenvalue Sum on Geometry Matrix
31. Harmonic Oscillator Model of Aromaticity Index
32. Jug Ring Current Index
33. Aromaticity Index
34. Homeostasis Model Assessment (HOMA) Total Index
35. CoMMA Displacement (Atomic Masses)
36. CoMMA Quadrupole XX (Atomic Masses)
37. CoMMA Quadrupole YY (Atomic Masses)
38. CoMMA Quadrupole ZZ (Atomic Masses)
39. CoMMA Displacement (Atomic van der Waals Volumes)
40. CoMMA Quadrupole XX (Atomic van der Waals Volumes)
41. CoMMA Quadrupole YY (Atomic van der Waals Volumes)
42. CoMMA Quadrupole ZZ (Atomic van der Waals Volumes)
43. CoMMA Displacement (Atomic Sanderson Electronegativities)
44. CoMMA Quadrupole XX (Atomic Sanderson Electronegativities)
45. CoMMA Quadrupole YY (Atomic Sanderson Electronegativities)
46. CoMMA Quadrupole ZZ (Atomic Sanderson Electronegativities)
47. CoMMA Displacement (Atomic Polarizabilities)
48. CoMMA Quadrupole XX (Atomic Polarizabilities)
49. CoMMA Quadrupole YY (Atomic Polarizabilities)
50. CoMMA Quadrupole ZZ (Atomic Polarizabilities)
51. Sum of Geometrical Distances Between N..N
52. Sum of Geometrical Distances Between N..O
53. Sum of Geometrical Distances Between N..S
54. Sum of Geometrical Distances Between O..O
55. Sum of Geometrical Distances Between O..S
56. Sum of Geometrical Distances Between S..S

RDF Descriptors

1. RDF S10 (Unweighted)
2. RDF S15 (Unweighted)
3. RDF S20 (Unweighted)
4. RDF S25 (Unweighted)
5. RDF S30 (Unweighted)
6. RDF S35 (Unweighted)
7. RDF S40 (Unweighted)
8. RDF S45 (Unweighted)

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9. RDF S50 (Unweighted)
10. RDF S55 (Unweighted)
11. RDF S60 (Unweighted)
12. RDF S65 (Unweighted)
13. RDF S70 (Unweighted)
14. RDF S75 (Unweighted)
15. RDF S80 (Unweighted)
16. RDF S85 (Unweighted)
17. RDF S90 (Unweighted)
18. RDF S95 (Unweighted)
19. RDF S100 (Unweighted)
20. RDF S105 (Unweighted)
21. RDF S110 (Unweighted)
22. RDF S115 (Unweighted)
23. RDF S120 (Unweighted)
24. RDF S125 (Unweighted)
25. RDF S130 (Unweighted)
26. RDF S135 (Unweighted)
27. RDF S140 (Unweighted)
28. RDF S145 (Unweighted)
29. RDF S150 (Unweighted)
30. RDF S155 (Unweighted)
31. RDF S10 (Atomic Masses)
32. RDF S15 (Atomic Masses)
33. RDF S20 (Atomic Masses)
34. RDF S25 (Atomic Masses)
35. RDF S30 (Atomic Masses)
36. RDF S35 (Atomic Masses)
37. RDF S40 (Atomic Masses)
38. RDF S45 (Atomic Masses)
39. RDF S50 (Atomic Masses)
40. RDF S55 (Atomic Masses)
41. RDF S60 (Atomic Masses)
42. RDF S65 (Atomic Masses)
43. RDF S70 (Atomic Masses)
44. RDF S75 (Atomic Masses)
45. RDF S80 (Atomic Masses)
46. RDF S85 (Atomic Masses)
47. RDF S90 (Atomic Masses)
48. RDF S95 (Atomic Masses)
49. RDF S100 (Atomic Masses)
50. RDF S105 (Atomic Masses)
51. RDF S110 (Atomic Masses)
52. RDF S115 (Atomic Masses)
53. RDF S120 (Atomic Masses)
54. RDF S125 (Atomic Masses)

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55. RDF S130 (Atomic Masses)
56. RDF S135 (Atomic Masses)
57. RDF S140 (Atomic Masses)
58. RDF S145 (Atomic Masses)
59. RDF S150 (Atomic Masses)
60. RDF S155 (Atomic Masses)
61. RDF S10 (Atomic van der Waals Volumes)
62. RDF S15 (Atomic van der Waals Volumes)
63. RDF S20 (Atomic van der Waals Volumes)
64. RDF S25 (Atomic van der Waals Volumes)
65. RDF S30 (Atomic van der Waals Volumes)
66. RDF S35 (Atomic van der Waals Volumes)
67. RDF S40 (Atomic van der Waals Volumes)
68. RDF S45 (Atomic van der Waals Volumes)
69. RDF S50 (Atomic van der Waals Volumes)
70. RDF S55 (Atomic van der Waals Volumes)
71. RDF S60 (Atomic van der Waals Volumes)
72. RDF S65 (Atomic van der Waals Volumes)
73. RDF S70 (Atomic van der Waals Volumes)
74. RDF S75 (Atomic van der Waals Volumes)
75. RDF S80 (Atomic van der Waals Volumes)
76. RDF S85 (Atomic van der Waals Volumes)
77. RDF S90 (Atomic van der Waals Volumes)
78. RDF S95 (Atomic van der Waals Volumes)
79. RDF S100 (Atomic van der Waals Volumes)
80. RDF S105 (Atomic van der Waals Volumes)
81. RDF S110 (Atomic van der Waals Volumes)
82. RDF S115 (Atomic van der Waals Volumes)
83. RDF S120 (Atomic van der Waals Volumes)
84. RDF S125 (Atomic van der Waals Volumes)
85. RDF S130 (Atomic van der Waals Volumes)
86. RDF S135 (Atomic van der Waals Volumes)
87. RDF S140 (Atomic van der Waals Volumes)
88. RDF S145 (Atomic van der Waals Volumes)
89. RDF S150 (Atomic van der Waals Volumes)
90. RDF S155 (Atomic van der Waals Volumes)
91. RDF S10 (Atomic Sanderson Electronegativities)
92. RDF S15 (Atomic Sanderson Electronegativities)
93. RDF S20 (Atomic Sanderson Electronegativities)
94. RDF S25 (Atomic Sanderson Electronegativities)
95. RDF S30 (Atomic Sanderson Electronegativities)
96. RDF S35 (Atomic Sanderson Electronegativities)
97. RDF S40 (Atomic Sanderson Electronegativities)
98. RDF S45 (Atomic Sanderson Electronegativities)
99. RDF S50 (Atomic Sanderson Electronegativities)
100. RDF S55 (Atomic Sanderson Electronegativities)

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101. RDF S60 (Atomic Sanderson Electronegativities)
102. RDF S65 (Atomic Sanderson Electronegativities)
103. RDF S70 (Atomic Sanderson Electronegativities)
104. RDF S75 (Atomic Sanderson Electronegativities)
105. RDF S80 (Atomic Sanderson Electronegativities)
106. RDF S85 (Atomic Sanderson Electronegativities)
107. RDF S90 (Atomic Sanderson Electronegativities)
108. RDF S95 (Atomic Sanderson Electronegativities)
109. RDF S100 (Atomic Sanderson Electronegativities)
110. RDF S105 (Atomic Sanderson Electronegativities)
111. RDF S110 (Atomic Sanderson Electronegativities)
112. RDF S115 (Atomic Sanderson Electronegativities)
113. RDF S120 (Atomic Sanderson Electronegativities)
114. RDF S125 (Atomic Sanderson Electronegativities)
115. RDF S130 (Atomic Sanderson Electronegativities)
116. RDF S135 (Atomic Sanderson Electronegativities)
117. RDF S140 (Atomic Sanderson Electronegativities)
118. RDF S145 (Atomic Sanderson Electronegativities)
119. RDF S150 (Atomic Sanderson Electronegativities)
120. RDF S155 (Atomic Sanderson Electronegativities)
121. RDF S10 (Atomic Polarizabilities)
122. RDF S15 (Atomic Polarizabilities)
123. RDF S20 (Atomic Polarizabilities)
124. RDF S25 (Atomic Polarizabilities)
125. RDF S30 (Atomic Polarizabilities)
126. RDF S35 (Atomic Polarizabilities)
127. RDF S40 (Atomic Polarizabilities)
128. RDF S45 (Atomic Polarizabilities)
129. RDF S50 (Atomic Polarizabilities)
130. RDF S55 (Atomic Polarizabilities)
131. RDF S60 (Atomic Polarizabilities)
132. RDF S65 (Atomic Polarizabilities)
133. RDF S70 (Atomic Polarizabilities)
134. RDF S75 (Atomic Polarizabilities)
135. RDF S80 (Atomic Polarizabilities)
136. RDF S85 (Atomic Polarizabilities)
137. RDF S90 (Atomic Polarizabilities)
138. RDF S95 (Atomic Polarizabilities)
139. RDF S100 (Atomic Polarizabilities)
140. RDF S105 (Atomic Polarizabilities)
141. RDF S110 (Atomic Polarizabilities)
142. RDF S115 (Atomic Polarizabilities)
143. RDF S120 (Atomic Polarizabilities)
144. RDF S125 (Atomic Polarizabilities)
145. RDF S130 (Atomic Polarizabilities)
146. RDF S135 (Atomic Polarizabilities)

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147. RDF S140 (Atomic Polarizabilities)
148. RDF S145 (Atomic Polarizabilities)
149. RDF S150 (Atomic Polarizabilities)
150. RDF S155 (Atomic Polarizabilities)

3D-MoRSE Descriptors

1. 3D-MoRSE S1 (Unweighted)
2. 3D-MoRSE S2 (Unweighted)
3. 3D-MoRSE S3 (Unweighted)
4. 3D-MoRSE S4 (Unweighted)
5. 3D-MoRSE S5 (Unweighted)
6. 3D-MoRSE S6 (Unweighted)
7. 3D-MoRSE S7 (Unweighted)
8. 3D-MoRSE S8 (Unweighted)
9. 3D-MoRSE S9 (Unweighted)
10. 3D-MoRSE S10 (Unweighted)
11. 3D-MoRSE S11 (Unweighted)
12. 3D-MoRSE S12 (Unweighted)
13. 3D-MoRSE S13 (Unweighted)
14. 3D-MoRSE S14 (Unweighted)
15. 3D-MoRSE S15 (Unweighted)
16. 3D-MoRSE S16 (Unweighted)
17. 3D-MoRSE S17 (Unweighted)
18. 3D-MoRSE S18 (Unweighted)
19. 3D-MoRSE S19 (Unweighted)
20. 3D-MoRSE S20 (Unweighted)
21. 3D-MoRSE S21 (Unweighted)
22. 3D-MoRSE S22 (Unweighted)
23. 3D-MoRSE S23 (Unweighted)
24. 3D-MoRSE S24 (Unweighted)
25. 3D-MoRSE S25 (Unweighted)
26. 3D-MoRSE S26 (Unweighted)
27. 3D-MoRSE S27 (Unweighted)
28. 3D-MoRSE S28 (Unweighted)
29. 3D-MoRSE S29 (Unweighted)
30. 3D-MoRSE S30 (Unweighted)
31. 3D-MoRSE S31 (Unweighted)
32. 3D-MoRSE S32 (Unweighted)
33. 3D-MoRSE S1 (Atomic Masses)
34. 3D-MoRSE S2 (Atomic Masses)
35. 3D-MoRSE S3 (Atomic Masses)
36. 3D-MoRSE S4 (Atomic Masses)
37. 3D-MoRSE S5 (Atomic Masses)
38. 3D-MoRSE S6 (Atomic Masses)
39. 3D-MoRSE S7 (Atomic Masses)

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40. 3D-MoRSE S8 (Atomic Masses)
41. 3D-MoRSE S9 (Atomic Masses)
42. 3D-MoRSE S10 (Atomic Masses)
43. 3D-MoRSE S11 (Atomic Masses)
44. 3D-MoRSE S12 (Atomic Masses)
45. 3D-MoRSE S13 (Atomic Masses)
46. 3D-MoRSE S14 (Atomic Masses)
47. 3D-MoRSE S15 (Atomic Masses)
48. 3D-MoRSE S16 (Atomic Masses)
49. 3D-MoRSE S17 (Atomic Masses)
50. 3D-MoRSE S18 (Atomic Masses)
51. 3D-MoRSE S19 (Atomic Masses)
52. 3D-MoRSE S20 (Atomic Masses)
53. 3D-MoRSE S21 (Atomic Masses)
54. 3D-MoRSE S22 (Atomic Masses)
55. 3D-MoRSE S23 (Atomic Masses)
56. 3D-MoRSE S24 (Atomic Masses)
57. 3D-MoRSE S25 (Atomic Masses)
58. 3D-MoRSE S26 (Atomic Masses)
59. 3D-MoRSE S27 (Atomic Masses)
60. 3D-MoRSE S28 (Atomic Masses)
61. 3D-MoRSE S29 (Atomic Masses)
62. 3D-MoRSE S30 (Atomic Masses)
63. 3D-MoRSE S31 (Atomic Masses)
64. 3D-MoRSE S32 (Atomic Masses)
65. 3D-MoRSE S1 (Atomic van der Waals Volumes)
66. 3D-MoRSE S2 (Atomic van der Waals Volumes)
67. 3D-MoRSE S3 (Atomic van der Waals Volumes)
68. 3D-MoRSE S4 (Atomic van der Waals Volumes)
69. 3D-MoRSE S5 (Atomic van der Waals Volumes)
70. 3D-MoRSE S6 (Atomic van der Waals Volumes)
71. 3D-MoRSE S7 (Atomic van der Waals Volumes)
72. 3D-MoRSE S8 (Atomic van der Waals Volumes)
73. 3D-MoRSE S9 (Atomic van der Waals Volumes)
74. 3D-MoRSE S10 (Atomic van der Waals Volumes)
75. 3D-MoRSE S11 (Atomic van der Waals Volumes)
76. 3D-MoRSE S12 (Atomic van der Waals Volumes)
77. 3D-MoRSE S13 (Atomic van der Waals Volumes)
78. 3D-MoRSE S14 (Atomic van der Waals Volumes)
79. 3D-MoRSE S15 (Atomic van der Waals Volumes)
80. 3D-MoRSE S16 (Atomic van der Waals Volumes)
81. 3D-MoRSE S17 (Atomic van der Waals Volumes)
82. 3D-MoRSE S18 (Atomic van der Waals Volumes)
83. 3D-MoRSE S19 (Atomic van der Waals Volumes)
84. 3D-MoRSE S20 (Atomic van der Waals Volumes)
85. 3D-MoRSE S21 (Atomic van der Waals Volumes)

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86. 3D-MoRSE S22 (Atomic van der Waals Volumes)
87. 3D-MoRSE S23 (Atomic van der Waals Volumes)
88. 3D-MoRSE S24 (Atomic van der Waals Volumes)
89. 3D-MoRSE S25 (Atomic van der Waals Volumes)
90. 3D-MoRSE S26 (Atomic van der Waals Volumes)
91. 3D-MoRSE S27 (Atomic van der Waals Volumes)
92. 3D-MoRSE S28 (Atomic van der Waals Volumes)
93. 3D-MoRSE S29 (Atomic van der Waals Volumes)
94. 3D-MoRSE S30 (Atomic van der Waals Volumes)
95. 3D-MoRSE S31 (Atomic van der Waals Volumes)
96. 3D-MoRSE S32 (Atomic van der Waals Volumes)
97. 3D-MoRSE S1 (Atomic Sanderson Electronegativities)
98. 3D-MoRSE S2 (Atomic Sanderson Electronegativities)
99. 3D-MoRSE S3 (Atomic Sanderson Electronegativities)
100. 3D-MoRSE S4 (Atomic Sanderson Electronegativities)
101. 3D-MoRSE S5 (Atomic Sanderson Electronegativities)
102. 3D-MoRSE S6 (Atomic Sanderson Electronegativities)
103. 3D-MoRSE S7 (Atomic Sanderson Electronegativities)
104. 3D-MoRSE S8 (Atomic Sanderson Electronegativities)
105. 3D-MoRSE S9 (Atomic Sanderson Electronegativities)
106. 3D-MoRSE S10 (Atomic Sanderson Electronegativities)
107. 3D-MoRSE S11 (Atomic Sanderson Electronegativities)
108. 3D-MoRSE S12 (Atomic Sanderson Electronegativities)
109. 3D-MoRSE S13 (Atomic Sanderson Electronegativities)
110. 3D-MoRSE S14 (Atomic Sanderson Electronegativities)
111. 3D-MoRSE S15 (Atomic Sanderson Electronegativities)
112. 3D-MoRSE S16 (Atomic Sanderson Electronegativities)
113. 3D-MoRSE S17 (Atomic Sanderson Electronegativities)
114. 3D-MoRSE S18 (Atomic Sanderson Electronegativities)
115. 3D-MoRSE S19 (Atomic Sanderson Electronegativities)
116. 3D-MoRSE S20 (Atomic Sanderson Electronegativities)
117. 3D-MoRSE S21 (Atomic Sanderson Electronegativities)
118. 3D-MoRSE S22 (Atomic Sanderson Electronegativities)
119. 3D-MoRSE S23 (Atomic Sanderson Electronegativities)
120. 3D-MoRSE S24 (Atomic Sanderson Electronegativities)
121. 3D-MoRSE S25 (Atomic Sanderson Electronegativities)
122. 3D-MoRSE S26 (Atomic Sanderson Electronegativities)
123. 3D-MoRSE S27 (Atomic Sanderson Electronegativities)
124. 3D-MoRSE S28 (Atomic Sanderson Electronegativities)
125. 3D-MoRSE S29 (Atomic Sanderson Electronegativities)
126. 3D-MoRSE S30 (Atomic Sanderson Electronegativities)
127. 3D-MoRSE S31 (Atomic Sanderson Electronegativities)
128. 3D-MoRSE S32 (Atomic Sanderson Electronegativities)
129. 3D-MoRSE S1 (Atomic Polarizabilities)
130. 3D-MoRSE S2 (Atomic Polarizabilities)
131. 3D-MoRSE S3 (Atomic Polarizabilities)

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132. 3D-MoRSE S4 (Atomic Polarizabilities)
133. 3D-MoRSE S5 (Atomic Polarizabilities)
134. 3D-MoRSE S6 (Atomic Polarizabilities)
135. 3D-MoRSE S7 (Atomic Polarizabilities)
136. 3D-MoRSE S8 (Atomic Polarizabilities)
137. 3D-MoRSE S9 (Atomic Polarizabilities)
138. 3D-MoRSE S10 (Atomic Polarizabilities)
139. 3D-MoRSE S11 (Atomic Polarizabilities)
140. 3D-MoRSE S12 (Atomic Polarizabilities)
141. 3D-MoRSE S13 (Atomic Polarizabilities)
142. 3D-MoRSE S14 (Atomic Polarizabilities)
143. 3D-MoRSE S15 (Atomic Polarizabilities)
144. 3D-MoRSE S16 (Atomic Polarizabilities)
145. 3D-MoRSE S17 (Atomic Polarizabilities)
146. 3D-MoRSE S18 (Atomic Polarizabilities)
147. 3D-MoRSE S19 (Atomic Polarizabilities)
148. 3D-MoRSE S20 (Atomic Polarizabilities)
149. 3D-MoRSE S21 (Atomic Polarizabilities)
150. 3D-MoRSE S22 (Atomic Polarizabilities)
151. 3D-MoRSE S23 (Atomic Polarizabilities)
152. 3D-MoRSE S24 (Atomic Polarizabilities)
153. 3D-MoRSE S25 (Atomic Polarizabilities)
154. 3D-MoRSE S26 (Atomic Polarizabilities)
155. 3D-MoRSE S27 (Atomic Polarizabilities)
156. 3D-MoRSE S28 (Atomic Polarizabilities)
157. 3D-MoRSE S29 (Atomic Polarizabilities)
158. 3D-MoRSE S30 (Atomic Polarizabilities)
159. 3D-MoRSE S31 (Atomic Polarizabilities)
160. 3D-MoRSE S32 (Atomic Polarizabilities)

WHIM Descriptors

1. 1st Comp. Directional WHIM Size (Unweighted)
2. 2nd Comp. Directional WHIM Size (Unweighted)
3. 3rd Comp. Directional WHIM Size (Unweighted)
4. 1st Comp. Directional WHIM Shape (Unweighted)
5. 2nd Comp. Directional WHIM Shape (Unweighted)
6. 1st Comp. Directional WHIM Symmetry (Unweighted)
7. 2nd Comp. Directional WHIM Symmetry (Unweighted)
8. 3rd Comp. Directional WHIM Symmetry (Unweighted)
9. 1st Comp. Directional WHIM Accessibility (Unweighted)
10. 2nd Comp. Directional WHIM Accessibility (Unweighted)
11. 3rd Comp. Directional WHIM Accessibility (Unweighted)
12. 1st Comp. Directional WHIM Size (Atomic Masses)
13. 2nd Comp. Directional WHIM Size (Atomic Masses)
14. 3rd Comp. Directional WHIM Size (Atomic Masses)

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15. 1st Comp. Directional WHIM Shape (Atomic Masses)
16. 2nd Comp. Directional WHIM Shape (Atomic Masses)
17. 1st Comp. Directional WHIM Symmetry (Atomic Masses)
18. 2nd Comp. Directional WHIM Symmetry (Atomic Masses)
19. 3rd Comp. Directional WHIM Symmetry (Atomic Masses)
20. 1st Comp. Directional WHIM Accessibility (Atomic Masses)
21. 2nd Comp. Directional WHIM Accessibility (Atomic Masses)
22. 3rd Comp. Directional WHIM Accessibility (Atomic Masses)
23. 1st Comp. Directional WHIM Size (Atomic van der Waals Volumes)
24. 2nd Comp. Directional WHIM Size (Atomic van der Waals Volumes)
25. 3rd Comp. Directional WHIM Size (Atomic van der Waals Volumes)
26. 1st Comp. Directional WHIM Shape (Atomic van der Waals Volumes)
27. 2nd Comp. Directional WHIM Shape (Atomic van der Waals Volumes)
28. 1st Comp. Directional WHIM Symmetry (Atomic van der Waals Volumes)
29. 2nd Comp. Directional WHIM Symmetry (Atomic van der Waals Volumes)
30. 3rd Comp. Directional WHIM Symmetry (Atomic van der Waals Volumes)
31. 1st Comp. Directional WHIM Accessibility (Atomic van der Waals Volumes)
32. 2nd Comp. Directional WHIM Accessibility (Atomic van der Waals Volumes)
33. 3rd Comp. Directional WHIM Accessibility (Atomic van der Waals Volumes)
34. 1st Comp. Directional WHIM Size (Atomic Sanderson Electronegativities)
35. 2nd Comp. Directional WHIM Size (Atomic Sanderson Electronegativities)
36. 3rd Comp. Directional WHIM Size (Atomic Sanderson Electronegativities)
37. 1st Comp. Directional WHIM Shape (Atomic Sanderson Electronegativities)
38. 2nd Comp. Directional WHIM Shape (Atomic Sanderson Electronegativities)
39. 1st Comp. Directional WHIM Symmetry (Atomic Sanderson Electronegativities)
40. 2nd Comp. Directional WHIM Symmetry (Atomic Sanderson Electronegativities)
41. 3rd Comp. Directional WHIM Symmetry (Atomic Sanderson Electronegativities)
42. 1st Comp. Directional WHIM Accessibility (Atomic Sanderson Electronegativities)
43. 2nd Comp. Directional WHIM Accessibility (Atomic Sanderson Electronegativities)
44. 3rd Comp. Directional WHIM Accessibility (Atomic Sanderson Electronegativities)
45. 1st Comp. Directional WHIM Size (Atomic Polarizabilities)
46. 2nd Comp. Directional WHIM Size (Atomic Polarizabilities)
47. 3rd Comp. Directional WHIM Size (Atomic Polarizabilities)
48. 1st Comp. Directional WHIM Shape (Atomic Polarizabilities)
49. 2nd Comp. Directional WHIM Shape (Atomic Polarizabilities)
50. 1st Comp. Directional WHIM Symmetry (Atomic Polarizabilities)
51. 2nd Comp. Directional WHIM Symmetry (Atomic Polarizabilities)
52. 3rd Comp. Directional WHIM Symmetry (Atomic Polarizabilities)
53. 1st Comp. Directional WHIM Accessibility (Atomic Polarizabilities)
54. 2nd Comp. Directional WHIM Accessibility (Atomic Polarizabilities)
55. 3rd Comp. Directional WHIM Accessibility (Atomic Polarizabilities)
56. 1st Comp. Directional WHIM Size (Atomic Electro-Topological States)
57. 2nd Comp. Directional WHIM Size (Atomic Electro-Topological States)
58. 3rd Comp. Directional WHIM Size (Atomic Electro-Topological States)
59. 1st Comp. Directional WHIM Shape (Atomic Electro-Topological States)
60. 2nd Comp. Directional WHIM Shape (Atomic Electro-Topological States)

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61. 1st Comp. Directional WHIM Symmetry (Atomic Electro-Topological States)
62. 2nd Comp. Directional WHIM Symmetry (Atomic Electro-Topological States)
63. 3rd Comp. Directional WHIM Symmetry (Atomic Electro-Topological States)
64. 1st Comp. Directional WHIM Accessibility (Atomic Electro-Topological States)
65. 2nd Comp. Directional WHIM Accessibility (Atomic Electro-Topological States)
66. 3rd Comp. Directional WHIM Accessibility (Atomic Electro-Topological States)
67. WHIM Total Size T (Unweighted)
68. WHIM Total Size T (Atomic Masses)
69. WHIM Total Size T (Atomic van der Waals Volumes)
70. WHIM Total Size T (Atomic Sanderson Electronegativities)
71. WHIM Total Size T (Atomic Polarizabilities)
72. WHIM Total Size T (Atomic Electro-Topological States)
73. WHIM Total Size A (Unweighted)
74. WHIM Total Size A (Atomic Masses)
75. WHIM Total Size A (Atomic van der Waals Volumes)
76. WHIM Total Size A (Atomic Sanderson Electronegativities)
77. WHIM Total Size A (Atomic Polarizabilities)
78. WHIM Total Size A (Atomic Electro-Topological States)
79. WHIM Total Symmetry (Unweighted)
80. WHIM Total Symmetry (Atomic Masses)
81. WHIM Total Symmetry (Atomic Electro-Topological States)
82. WHIM Global Shape (Unweighted)
83. WHIM Global Shape (Atomic Masses)
84. WHIM Global Shape (Atomic van der Waals Volumes)
85. WHIM Global Shape (Atomic Sanderson Electronegativities)
86. WHIM Global Shape (Atomic Polarizabilities)
87. WHIM Global Shape (Atomic Electro-Topological States)
88. WHIM Total Accessibility (Unweighted)
89. WHIM Total Accessibility (Atomic Masses)
90. WHIM Total Accessibility (Atomic van der Waals Volumes)
91. WHIM Total Accessibility (Atomic Sanderson Electronegativities)
92. WHIM Total Accessibility (Atomic Polarizabilities)
93. WHIM Total Accessibility (Atomic Electro-Topological States)
94. WHIM Total Size V (Unweighted)
95. WHIM Total Size V (Atomic Masses)
96. WHIM Total Size V (Atomic van der Waals Volumes)
97. WHIM Total Size V (Atomic Sanderson Electronegativities)
98. WHIM Total Size V (Atomic Polarizabilities)
99. WHIM Total Size V (Atomic Electro-Topological States)

GETAWAY Descriptors

1. GETAWAY Total Information Content
2. GETAWAY Standardized Information Content
3. GETAWAY Mean Information Content
4. GETAWAY Geometric Mean

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5. GETAWAY H K0 (Unweighted)
6. GETAWAY H K1 (Unweighted)
7. GETAWAY H K2 (Unweighted)
8. GETAWAY H K3 (Unweighted)
9. GETAWAY H K4 (Unweighted)
10. GETAWAY H K5 (Unweighted)
11. GETAWAY H K6 (Unweighted)
12. GETAWAY H K7 (Unweighted)
13. GETAWAY H K8 (Unweighted)
14. GETAWAY H Total (Unweighted)
15. GETAWAY HATS K0 (Unweighted)
16. GETAWAY HATS K1 (Unweighted)
17. GETAWAY HATS K2 (Unweighted)
18. GETAWAY HATS K3 (Unweighted)
19. GETAWAY HATS K4 (Unweighted)
20. GETAWAY HATS K5 (Unweighted)
21. GETAWAY HATS K6 (Unweighted)
22. GETAWAY HATS K7 (Unweighted)
23. GETAWAY HATS K8 (Unweighted)
24. GETAWAY HATS Total (Unweighted)
25. GETAWAY H K0 (Atomic Masses)
26. GETAWAY H K1 (Atomic Masses)
27. GETAWAY H K2 (Atomic Masses)
28. GETAWAY H K3 (Atomic Masses)
29. GETAWAY H K4 (Atomic Masses)
30. GETAWAY H K5 (Atomic Masses)
31. GETAWAY H K6 (Atomic Masses)
32. GETAWAY H K7 (Atomic Masses)
33. GETAWAY H K8 (Atomic Masses)
34. GETAWAY H Total (Atomic Masses)
35. GETAWAY HATS K0 (Atomic Masses)
36. GETAWAY HATS K1 (Atomic Masses)
37. GETAWAY HATS K2 (Atomic Masses)
38. GETAWAY HATS K3 (Atomic Masses)
39. GETAWAY HATS K4 (Atomic Masses)
40. GETAWAY HATS K5 (Atomic Masses)
41. GETAWAY HATS K6 (Atomic Masses)
42. GETAWAY HATS K7 (Atomic Masses)
43. GETAWAY HATS K8 (Atomic Masses)
44. GETAWAY HATS Total (Atomic Masses)
45. GETAWAY H K0 (Atomic van der Waals Volumes)
46. GETAWAY H K1 (Atomic van der Waals Volumes)
47. GETAWAY H K2 (Atomic van der Waals Volumes)
48. GETAWAY H K3 (Atomic van der Waals Volumes)
49. GETAWAY H K4 (Atomic van der Waals Volumes)
50. GETAWAY H K5 (Atomic van der Waals Volumes)

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51. GETAWAY H K6 (Atomic van der Waals Volumes)
52. GETAWAY H K7 (Atomic van der Waals Volumes)
53. GETAWAY H K8 (Atomic van der Waals Volumes)
54. GETAWAY H Total (Atomic van der Waals Volumes)
55. GETAWAY HATS K0 (Atomic van der Waals Volumes)
56. GETAWAY HATS K1 (Atomic van der Waals Volumes)
57. GETAWAY HATS K2 (Atomic van der Waals Volumes)
58. GETAWAY HATS K3 (Atomic van der Waals Volumes)
59. GETAWAY HATS K4 (Atomic van der Waals Volumes)
60. GETAWAY HATS K5 (Atomic van der Waals Volumes)
61. GETAWAY HATS K6 (Atomic van der Waals Volumes)
62. GETAWAY HATS K7 (Atomic van der Waals Volumes)
63. GETAWAY HATS K8 (Atomic van der Waals Volumes)
64. GETAWAY HATS Total (Atomic van der Waals Volumes)
65. GETAWAY H K0 (Atomic Sanderson Electronegativities)
66. GETAWAY H K1 (Atomic Sanderson Electronegativities)
67. GETAWAY H K2 (Atomic Sanderson Electronegativities)
68. GETAWAY H K3 (Atomic Sanderson Electronegativities)
69. GETAWAY H K4 (Atomic Sanderson Electronegativities)
70. GETAWAY H K5 (Atomic Sanderson Electronegativities)
71. GETAWAY H K6 (Atomic Sanderson Electronegativities)
72. GETAWAY H K7 (Atomic Sanderson Electronegativities)
73. GETAWAY H K8 (Atomic Sanderson Electronegativities)
74. GETAWAY H Total (Atomic Sanderson Electronegativities)
75. GETAWAY HATS K0 (Atomic Sanderson Electronegativities)
76. GETAWAY HATS K1 (Atomic Sanderson Electronegativities)
77. GETAWAY HATS K2 (Atomic Sanderson Electronegativities)
78. GETAWAY HATS K3 (Atomic Sanderson Electronegativities)
79. GETAWAY HATS K4 (Atomic Sanderson Electronegativities)
80. GETAWAY HATS K5 (Atomic Sanderson Electronegativities)
81. GETAWAY HATS K6 (Atomic Sanderson Electronegativities)
82. GETAWAY HATS K7 (Atomic Sanderson Electronegativities)
83. GETAWAY HATS K8 (Atomic Sanderson Electronegativities)
84. GETAWAY HATS Total (Atomic Sanderson Electronegativities)
85. GETAWAY H K0 (Atomic Polarizabilities)
86. GETAWAY H K1 (Atomic Polarizabilities)
87. GETAWAY H K2 (Atomic Polarizabilities)
88. GETAWAY H K3 (Atomic Polarizabilities)
89. GETAWAY H K4 (Atomic Polarizabilities)
90. GETAWAY H K5 (Atomic Polarizabilities)
91. GETAWAY H K6 (Atomic Polarizabilities)
92. GETAWAY H K7 (Atomic Polarizabilities)
93. GETAWAY H K8 (Atomic Polarizabilities)
94. GETAWAY H Total (Atomic Polarizabilities)
95. GETAWAY HATS K0 (Atomic Polarizabilities)
96. GETAWAY HATS K1 (Atomic Polarizabilities)

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97. GETAWAY HATS K2 (Atomic Polarizabilities)
98. GETAWAY HATS K3 (Atomic Polarizabilities)
99. GETAWAY HATS K4 (Atomic Polarizabilities)
100. GETAWAY HATS K5 (Atomic Polarizabilities)
101. GETAWAY HATS K6 (Atomic Polarizabilities)
102. GETAWAY HATS K7 (Atomic Polarizabilities)
103. GETAWAY HATS K8 (Atomic Polarizabilities)
104. GETAWAY HATS Total (Atomic Polarizabilities)
105. GETAWAY R Matrix Connectivity
106. GETAWAY R Matrix Avg Row Sum
107. GETAWAY R Matrix 1st Eigenvalue
108. GETAWAY R K1 (Unweighted)
109. GETAWAY R K2 (Unweighted)
110. GETAWAY R K3 (Unweighted)
111. GETAWAY R K4 (Unweighted)
112. GETAWAY R K5 (Unweighted)
113. GETAWAY R K6 (Unweighted)
114. GETAWAY R K7 (Unweighted)
115. GETAWAY R K8 (Unweighted)
116. GETAWAY R Total (Unweighted)
117. GETAWAY R Max K1 (Unweighted)
118. GETAWAY R Max K2 (Unweighted)
119. GETAWAY R Max K3 (Unweighted)
120. GETAWAY R Max K4 (Unweighted)
121. GETAWAY R Max K5 (Unweighted)
122. GETAWAY R Max K6 (Unweighted)
123. GETAWAY R Max K7 (Unweighted)
124. GETAWAY R Max K8 (Unweighted)
125. GETAWAY R Max (Unweighted)
126. GETAWAY R K1 (Atomic Masses)
127. GETAWAY R K2 (Atomic Masses)
128. GETAWAY R K3 (Atomic Masses)
129. GETAWAY R K4 (Atomic Masses)
130. GETAWAY R K5 (Atomic Masses)
131. GETAWAY R K6 (Atomic Masses)
132. GETAWAY R K7 (Atomic Masses)
133. GETAWAY R K8 (Atomic Masses)
134. GETAWAY R Total (Atomic Masses)
135. GETAWAY R Max K1 (Atomic Masses)
136. GETAWAY R Max K2 (Atomic Masses)
137. GETAWAY R Max K3 (Atomic Masses)
138. GETAWAY R Max K4 (Atomic Masses)
139. GETAWAY R Max K5 (Atomic Masses)
140. GETAWAY R Max K6 (Atomic Masses)
141. GETAWAY R Max K7 (Atomic Masses)
142. GETAWAY R Max K8 (Atomic Masses)

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143. GETAWAY R Max (Atomic Masses)
144. GETAWAY R K1 (Atomic van der Waals Volumes)
145. GETAWAY R K2 (Atomic van der Waals Volumes)
146. GETAWAY R K3 (Atomic van der Waals Volumes)
147. GETAWAY R K4 (Atomic van der Waals Volumes)
148. GETAWAY R K5 (Atomic van der Waals Volumes)
149. GETAWAY R K6 (Atomic van der Waals Volumes)
150. GETAWAY R K7 (Atomic van der Waals Volumes)
151. GETAWAY R K8 (Atomic van der Waals Volumes)
152. GETAWAY R Total (Atomic van der Waals Volumes)
153. GETAWAY R Max K1 (Atomic van der Waals Volumes)
154. GETAWAY R Max K2 (Atomic van der Waals Volumes)
155. GETAWAY R Max K3 (Atomic van der Waals Volumes)
156. GETAWAY R Max K4 (Atomic van der Waals Volumes)
157. GETAWAY R Max K5 (Atomic van der Waals Volumes)
158. GETAWAY R Max K6 (Atomic van der Waals Volumes)
159. GETAWAY R Max K7 (Atomic van der Waals Volumes)
160. GETAWAY R Max K8 (Atomic van der Waals Volumes)
161. GETAWAY R Max (Atomic van der Waals Volumes)
162. GETAWAY R K1 (Atomic Sanderson Electronegativities)
163. GETAWAY R K2 (Atomic Sanderson Electronegativities)
164. GETAWAY R K3 (Atomic Sanderson Electronegativities)
165. GETAWAY R K4 (Atomic Sanderson Electronegativities)
166. GETAWAY R K5 (Atomic Sanderson Electronegativities)
167. GETAWAY R K6 (Atomic Sanderson Electronegativities)
168. GETAWAY R K7 (Atomic Sanderson Electronegativities)
169. GETAWAY R K8 (Atomic Sanderson Electronegativities)
170. GETAWAY R Total (Atomic Sanderson Electronegativities)
171. GETAWAY R Max K1 (Atomic Sanderson Electronegativities)
172. GETAWAY R Max K2 (Atomic Sanderson Electronegativities)
173. GETAWAY R Max K3 (Atomic Sanderson Electronegativities)
174. GETAWAY R Max K4 (Atomic Sanderson Electronegativities)
175. GETAWAY R Max K5 (Atomic Sanderson Electronegativities)
176. GETAWAY R Max K6 (Atomic Sanderson Electronegativities)
177. GETAWAY R Max K7 (Atomic Sanderson Electronegativities)
178. GETAWAY R Max K8 (Atomic Sanderson Electronegativities)
179. GETAWAY R Max (Atomic Sanderson Electronegativities)
180. GETAWAY R K1 (Atomic Polarizabilities)
181. GETAWAY R K2 (Atomic Polarizabilities)
182. GETAWAY R K3 (Atomic Polarizabilities)
183. GETAWAY R K4 (Atomic Polarizabilities)
184. GETAWAY R K5 (Atomic Polarizabilities)
185. GETAWAY R K6 (Atomic Polarizabilities)
186. GETAWAY R K7 (Atomic Polarizabilities)
187. GETAWAY R K8 (Atomic Polarizabilities)
188. GETAWAY R Total (Atomic Polarizabilities)

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189. GETAWAY R Max K1 (Atomic Polarizabilities)
190. GETAWAY R Max K2 (Atomic Polarizabilities)
191. GETAWAY R Max K3 (Atomic Polarizabilities)
192. GETAWAY R Max K4 (Atomic Polarizabilities)
193. GETAWAY R Max K5 (Atomic Polarizabilities)
194. GETAWAY R Max K6 (Atomic Polarizabilities)
195. GETAWAY R Max K7 (Atomic Polarizabilities)
196. GETAWAY R Max K8 (Atomic Polarizabilities)
197. GETAWAY R Max (Atomic Polarizabilities)

Functional Group Counts

1. Number of Terminal Primary C(sp3)
2. Number of Total Secondary C(sp3)
3. Number of Total Tertiary C(sp3)
4. Number of Total Quaternary C(sp3)
5. Number of Ring Secondary C(sp3)
6. Number of Ring Tertiary C(sp3)
7. Number of Ring Quaternary C(sp3)
8. Number of Aromatic C(sp2)
9. Number of Unsubstituted Benzene C(sp2)
10. Number of Substituted Benzene C(sp2)
11. Number of Non-Aromatic Conjugated C(sp2)
12. Number of Terminal Primary C(sp2)
13. Number of Aliphatic Secondary C(sp2)
14. Number of Aliphatic Tertiary C(sp2)
15. Number of Allenes Groups
16. Number of Terminal C(sp)
17. Number of Non-Terminal C(sp)
18. Number of Cyanates (Aliphatic)
19. Number of Cyanates (Aromatic)
20. Number of Isocyanates (Aliphatic)
21. Number of Isocyanates (Aromatic)
22. Number of Thiocyanates (Aliphatic)
23. Number of Thiocyanates (Aromatic)
24. Number of Isothiocyanates (Aliphatic)
25. Number of Isothiocyanates (Aromatic)
26. Number of Carboxylic Acids (Aliphatic)
27. Number of Carboxylic Acids (Aromatic)
28. Number of Esters (Aliphatic)
29. Number of Esters (Aromatic)
30. Number of Primary Amides (Aliphatic)
31. Number of Primary Amides (Aromatic)
32. Number of Secondary Amides (Aliphatic)
33. Number of Secondary Amides (Aromatic)
34. Number of Tertiary Amides (Aliphatic)

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35. Number of Tertiary Amides (Aromatic)
36. Number of (Thio-) Carbamates (Aliphatic)
37. Number of (Thio-) Carbamates (Aromatic)
38. Number of Thioacids (Aliphatic)
39. Number of Thioacids (Aromatic)
40. Number of Dithioacids (Aliphatic)
41. Number of Dithioacids (Aromatic)
42. Number of Thioesters (Aliphatic)
43. Number of Thioesters (Aromatic)
44. Number of Dithioesters (Aliphatic)
45. Number of Dithioesters (Aromatic)
46. Number of Aldehydes (Aliphatic)
47. Number of Aldehydes (Aromatic)
48. Number of Ketones (Aliphatic)
49. Number of Ketones (Aromatic)
50. Number of Urea (-Thio) Derivatives
51. Number of Carbonate (-Thio) Derivatives
52. Number of Amidine Derivatives
53. Number of Guanidine Derivatives
54. Number of Imines (Aliphatic)
55. Number of Imines (Aromatic)
56. Number of Oximes (Aliphatic)
57. Number of Oximes (Aromatic)
58. Number of Primary Amines (Aliphatic)
59. Number of Primary Amines (Aromatic)
60. Number of Secondary Amines (Aliphatic)
61. Number of Secondary Amines (Aromatic)
62. Number of Tertiary Amines (Aliphatic)
63. Number of Tertiary Amines (Aromatic)
64. Number of N Hydrazines
65. Number of N Azo-Derivatives
66. Number of Nitriles (Aliphatic)
67. Number of Nitriles (Aromatic)
68. Number of Positively Charged N
69. Number of Quaternary N
70. Number of Hydroxylamines (Aliphatic)
71. Number of Hydroxylamines (Aromatic)
72. Number of N-Nitroso Groups (Aliphatic)
73. Number of N-Nitroso Groups (Aromatic)
74. Number of Nitroso Groups (Aliphatic)
75. Number of Nitroso Groups (Aromatic)
76. Number of Nitro Groups (Aliphatic)
77. Number of Nitro Groups (Aromatic)
78. Number of Imides
79. Number of Hydrazones
80. Number of Hydroxyl Groups

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81. Number of Aromatic Hydroxyls
82. Number of Primary Alcohols
83. Number of Secondary Alcohols
84. Number of Tertiary Alcohols
85. Number of Ethers (Aliphatic)
86. Number of Ethers (Aromatic)
87. Number of Anhydrides (Thio-)
88. Number of Water Molecules
89. Number of Thiols
90. Number of Thioketones
91. Number of Sulfides
92. Number of Disulfides
93. Number of Sulfoxides
94. Number of Sulfones
95. Number of Sulfenic (Thio-) Acids
96. Number of Sulfinic (Thio-/Dithio-) Acids
97. Number of Sulfonic (Thio-/Dithio-) Acids
98. Number of Sulfuric (Thio-/Dithio-) Acids
99. Number of Sulfites (Thio-/Dithio-)
100. Number of Sulfonates (Thio-/Dithio-)
101. Number of Sulfates (Thio-/Dithio-)
102. Number of Sulfonamides/Sulfinamides/Sulfenamides (Thio-/Dithio-)
103. Number of Aziridines
104. Number of Oxiranes
105. Number of Thiranes
106. Number of Azetidines
107. Number of Oxetanes
108. Number of Thioethanes
109. Number of Pyrrolidines
110. Number of Oxolanes
111. Number of th-Thiophenes
112. Number of Pyrroles
113. Number of Pyrazoles
114. Number of Imidazoles
115. Number of Furanes
116. Number of Thiophenes
117. Number of Oxazoles
118. Number of Isoxazoles
119. Number of Thiazoles
120. Number of Isothiazoles
121. Number of Triazoles
122. Number of Pyridines
123. Number of Pyridazines
124. Number of Pyrimidines
125. Number of Pyrazines
126. Number of 135-Triazines

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127. Number of 124-Triazines
128. Number of Donor Atoms for H-Bonds (N and O)
129. Number of Acceptor Atoms for H-Bonds (N,O,F)
130. Number of Intramolecular H-Bonds

Atom-Centred Fragments

1. CH3R / CH4
2. CH2R2
3. CHR3
4. CR4
5. CH3X
6. CH2RX
7. CH2X2
8. CHR2X
9. CHRX2
10. CHX3
11. CR3X
12. CR2X2
13. CRX3
14. CX4
15. =CH2
16. =CHR
17. =CR2
18. =CHX
19. =CRX
20. =CX2
21. #CH
22. #CR / R=C=R
23. #CX
24. R--CH--R
25. R--CR--R
26. R--CX--R
27. R--CH--X
28. R--CR--X
29. R--CX--X
30. X--CH--X
31. X--CR--X
32. X--CX--X
33. R--CH..X
34. R--CR..X
35. R--CX..X
36. Al-CH=X
37. Ar-CH=X
38. Al-C(=X)-Al
39. Ar-C(=X)-R

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40. R-C(=X)-X / R-C#X / X=C=X
41. X-C(=X)-X
42. X--CH..X
43. X--CR..X
44. X--CX..X
45. H Attached to C0(sp3) no X Attached to Next C
46. H Attached to C1(sp3) / C0(sp2)
47. H Attached to C2(sp3) / C1(sp2) / C0(sp)
48. H Attached to C3(sp3) / C2(sp2) / C3(sp2) / C3(sp)
49. H Attached to Heteroatom
50. H Attached to Alpha-C
51. H Attached to C0(sp3) with 1X Attached to Next C
52. H Attached to C0(sp3) with 2X Attached to Next C
53. H Attached to C0(sp3) with 3X Attached to Next C
54. H Attached to C0(sp3) with 4X Attached to Next C
55. Alcohol
56. Phenol / Enol / Carboxyl OH
57. =O
58. Al-O-Al
59. Al-O-Ar / Ar-O-Ar / R..O..R / R-O-C=X
60. O--
61. R-O-O-R
62. Al-NH2
63. Al2-NH
64. Al3-N
65. Ar-NH2 / X-NH2
66. Ar-NH-Al
67. Ar-NAl2
68. RCO-N< / >N-X=X
69. Ar2NH / Ar3N / Ar2N-Al / R..N..R
70. R#N / R=N-
71. R--N--R / R--N--X
72. Ar-NO2 / R--N(--R)--O / RO-NO
73. Al-NO2
74. Ar-N=X / X-N=X
75. N+ (Positively Charged)
76. R-SH
77. R2S / RS-SR
78. R=S
79. R-SO-R
80. R-SO2-R

Charge Descriptors

1. Maximum Positive Charge
2. Maximum Negative Charge

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3. Total Positive Charge
4. Total Negative Charge
5. Total Absolute Charge
6. Mean Absolute Charge
7. Total Squared Charge
8. Relative Positive Charge
9. Relative Negative Charge
10. Submolecular Polarity Parameter
11. Topological Electronic Descriptor
12. Topological Electronic Descriptor (Bond Restricted)
13. Partial Charge Weighted Topological Electronic Descriptor
14. Local Dipole Index

Molecular Properties

1. Unsaturation Index
2. Hydrophilic Factor
3. Ghose-Crippen Molar Refractivity
4. Fragment-Based Polar Surface Area from N,O Polar Coefficients)
5. Fragment-Based Polar Surface Area from N,O,S,P Polar Coefficients)
6. Moriguchi Octanol-Water Partition Coefficient (Mlogp)
7. Squared Moriguchi Octanol-Water Partition Coefficient (Mlogp^2)
8. Ghose-Crippen Octanol-Water Partition Coefficient (Alogp)
9. Squared Ghose-Crippen Octanol-Water Partition Coefficient (Alogp^2)
10. Lipinski Alert Index
11. Ghose-Viswanadhan-Wendoloski Drug-Like (Covering 80%)
12. Ghose-Viswanadhan-Wendoloski Drug-Like (Covering 50%)
13. Ghose-Viswanadhan-Wendoloski Antiinflammatory (Covering 80%)
14. Ghose-Viswanadhan-Wendoloski Antiinflammatory (Covering 50%)
15. Ghose-Viswanadhan-Wendoloski Antidepressant (Covering 80%)
16. Ghose-Viswanadhan-Wendoloski Antidepressant (Covering 50%)
17. Ghose-Viswanadhan-Wendoloski Antipsychotic (Covering 80%)
18. Ghose-Viswanadhan-Wendoloski Antipsychotic (Covering 50%)
19. Ghose-Viswanadhan-Wendoloski Antihypertensive (Covering 80%)
20. Ghose-Viswanadhan-Wendoloski Antihypertensive (Covering 50%)
21. Ghose-Viswanadhan-Wendoloski Hypnotic (Covering 80%)
22. Ghose-Viswanadhan-Wendoloski Hypnotic (Covering 50%)
23. Ghose-Viswanadhan-Wendoloski Antineoplastic (Covering 80%)
24. Ghose-Viswanadhan-Wendoloski Antineoplastic (Covering 50%)
25. Ghose-Viswanadhan-Wendoloski Antiinfective (Covering 80%)
26. Ghose-Viswanadhan-Wendoloski Antiinfective (Covering 50%)

2D Binary Fingerprints

1. Existence of C - C at Topological Distance 1
2. Existence of C - N at Topological Distance 1

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3. Existence of C - O at Topological Distance 1
4. Existence of C - S at Topological Distance 1
5. Existence of N - N at Topological Distance 1
6. Existence of N - O at Topological Distance 1
7. Existence of N - S at Topological Distance 1
8. Existence of O - O at Topological Distance 1
9. Existence of O - S at Topological Distance 1
10. Existence of S - S at Topological Distance 1
11. Existence of C - C at Topological Distance 2
12. Existence of C - N at Topological Distance 2
13. Existence of C - O at Topological Distance 2
14. Existence of C - S at Topological Distance 2
15. Existence of N - N at Topological Distance 2
16. Existence of N - O at Topological Distance 2
17. Existence of N - S at Topological Distance 2
18. Existence of O - O at Topological Distance 2
19. Existence of O - S at Topological Distance 2
20. Existence of S - S at Topological Distance 2
21. Existence of C - C at Topological Distance 3
22. Existence of C - N at Topological Distance 3
23. Existence of C - O at Topological Distance 3
24. Existence of C - S at Topological Distance 3
25. Existence of N - N at Topological Distance 3
26. Existence of N - O at Topological Distance 3
27. Existence of N - S at Topological Distance 3
28. Existence of O - O at Topological Distance 3
29. Existence of O - S at Topological Distance 3
30. Existence of S - S at Topological Distance 3
31. Existence of C - C at Topological Distance 4
32. Existence of C - N at Topological Distance 4
33. Existence of C - O at Topological Distance 4
34. Existence of C - S at Topological Distance 4
35. Existence of N - N at Topological Distance 4
36. Existence of N - O at Topological Distance 4
37. Existence of N - S at Topological Distance 4
38. Existence of O - O at Topological Distance 4
39. Existence of O - S at Topological Distance 4
40. Existence of S - S at Topological Distance 4
41. Existence of C - C at Topological Distance 5
42. Existence of C - N at Topological Distance 5
43. Existence of C - O at Topological Distance 5
44. Existence of C - S at Topological Distance 5
45. Existence of N - N at Topological Distance 5
46. Existence of N - O at Topological Distance 5
47. Existence of N - S at Topological Distance 5
48. Existence of O - O at Topological Distance 5

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49. Existence of O - S at Topological Distance 5
50. Existence of S - S at Topological Distance 5
51. Existence of C - C at Topological Distance 6
52. Existence of C - N at Topological Distance 6
53. Existence of C - O at Topological Distance 6
54. Existence of C - S at Topological Distance 6
55. Existence of N - N at Topological Distance 6
56. Existence of N - O at Topological Distance 6
57. Existence of N - S at Topological Distance 6
58. Existence of O - O at Topological Distance 6
59. Existence of O - S at Topological Distance 6
60. Existence of S - S at Topological Distance 6
61. Existence of C - C at Topological Distance 7
62. Existence of C - N at Topological Distance 7
63. Existence of C - O at Topological Distance 7
64. Existence of C - S at Topological Distance 7
65. Existence of N - N at Topological Distance 7
66. Existence of N - O at Topological Distance 7
67. Existence of N - S at Topological Distance 7
68. Existence of O - O at Topological Distance 7
69. Existence of O - S at Topological Distance 7
70. Existence of S - S at Topological Distance 7
71. Existence of C - C at Topological Distance 8
72. Existence of C - N at Topological Distance 8
73. Existence of C - O at Topological Distance 8
74. Existence of C - S at Topological Distance 8
75. Existence of N - N at Topological Distance 8
76. Existence of N - O at Topological Distance 8
77. Existence of N - S at Topological Distance 8
78. Existence of O - O at Topological Distance 8
79. Existence of O - S at Topological Distance 8
80. Existence of S - S at Topological Distance 8
81. Existence of C - C at Topological Distance 9
82. Existence of C - N at Topological Distance 9
83. Existence of C - O at Topological Distance 9
84. Existence of C - S at Topological Distance 9
85. Existence of N - N at Topological Distance 9
86. Existence of N - O at Topological Distance 9
87. Existence of N - S at Topological Distance 9
88. Existence of O - O at Topological Distance 9
89. Existence of O - S at Topological Distance 9
90. Existence of S - S at Topological Distance 9
91. Existence of C - C at Topological Distance 10
92. Existence of C - N at Topological Distance 10
93. Existence of C - O at Topological Distance 10
94. Existence of C - S at Topological Distance 10

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95. Existence of N - N at Topological Distance 10
96. Existence of N - O at Topological Distance 10
97. Existence of N - S at Topological Distance 10
98. Existence of O - O at Topological Distance 10
99. Existence of O - S at Topological Distance 10
100. Existence of S - S at Topological Distance 10

2D Frequency Fingerprints

1. Frequency of C - C at Topological Distance 1
2. Frequency of C - N at Topological Distance 1
3. Frequency of C - O at Topological Distance 1
4. Frequency of C - S at Topological Distance 1
5. Frequency of N - N at Topological Distance 1
6. Frequency of N - O at Topological Distance 1
7. Frequency of N - S at Topological Distance 1
8. Frequency of O - O at Topological Distance 1
9. Frequency of O - S at Topological Distance 1
10. Frequency of S - S at Topological Distance 1
11. Frequency of C - C at Topological Distance 2
12. Frequency of C - N at Topological Distance 2
13. Frequency of C - O at Topological Distance 2
14. Frequency of C - S at Topological Distance 2
15. Frequency of N - N at Topological Distance 2
16. Frequency of N - O at Topological Distance 2
17. Frequency of N - S at Topological Distance 2
18. Frequency of O - O at Topological Distance 2
19. Frequency of O - S at Topological Distance 2
20. Frequency of S - S at Topological Distance 2
21. Frequency of C - C at Topological Distance 3
22. Frequency of C - N at Topological Distance 3
23. Frequency of C - O at Topological Distance 3
24. Frequency of C - S at Topological Distance 3
25. Frequency of N - N at Topological Distance 3
26. Frequency of N - O at Topological Distance 3
27. Frequency of N - S at Topological Distance 3
28. Frequency of O - O at Topological Distance 3
29. Frequency of O - S at Topological Distance 3
30. Frequency of S - S at Topological Distance 3
31. Frequency of C - C at Topological Distance 4
32. Frequency of C - N at Topological Distance 4
33. Frequency of C - O at Topological Distance 4
34. Frequency of C - S at Topological Distance 4
35. Frequency of N - N at Topological Distance 4
36. Frequency of N - O at Topological Distance 4
37. Frequency of N - S at Topological Distance 4

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38. Frequency of O - O at Topological Distance 4
39. Frequency of O - S at Topological Distance 4
40. Frequency of S - S at Topological Distance 4
41. Frequency of C - C at Topological Distance 5
42. Frequency of C - N at Topological Distance 5
43. Frequency of C - O at Topological Distance 5
44. Frequency of C - S at Topological Distance 5
45. Frequency of N - N at Topological Distance 5
46. Frequency of N - O at Topological Distance 5
47. Frequency of N - S at Topological Distance 5
48. Frequency of O - O at Topological Distance 5
49. Frequency of O - S at Topological Distance 5
50. Frequency of S - S at Topological Distance 5
51. Frequency of C - C at Topological Distance 6
52. Frequency of C - N at Topological Distance 6
53. Frequency of C - O at Topological Distance 6
54. Frequency of C - S at Topological Distance 6
55. Frequency of N - N at Topological Distance 6
56. Frequency of N - O at Topological Distance 6
57. Frequency of N - S at Topological Distance 6
58. Frequency of O - O at Topological Distance 6
59. Frequency of O - S at Topological Distance 6
60. Frequency of S - S at Topological Distance 6
61. Frequency of C - C at Topological Distance 7
62. Frequency of C - N at Topological Distance 7
63. Frequency of C - O at Topological Distance 7
64. Frequency of C - S at Topological Distance 7
65. Frequency of N - N at Topological Distance 7
66. Frequency of N - O at Topological Distance 7
67. Frequency of N - S at Topological Distance 7
68. Frequency of O - O at Topological Distance 7
69. Frequency of O - S at Topological Distance 7
70. Frequency of S - S at Topological Distance 7
71. Frequency of C - C at Topological Distance 8
72. Frequency of C - N at Topological Distance 8
73. Frequency of C - O at Topological Distance 8
74. Frequency of C - S at Topological Distance 8
75. Frequency of N - N at Topological Distance 8
76. Frequency of N - O at Topological Distance 8
77. Frequency of N - S at Topological Distance 8
78. Frequency of O - O at Topological Distance 8
79. Frequency of O - S at Topological Distance 8
80. Frequency of S - S at Topological Distance 8
81. Frequency of C - C at Topological Distance 9
82. Frequency of C - N at Topological Distance 9
83. Frequency of C - O at Topological Distance 9

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84. Frequency of C - S at Topological Distance 9
85. Frequency of N - N at Topological Distance 9
86. Frequency of N - O at Topological Distance 9
87. Frequency of N - S at Topological Distance 9
88. Frequency of O - O at Topological Distance 9
89. Frequency of O - S at Topological Distance 9
90. Frequency of S - S at Topological Distance 9
91. Frequency of C - C at Topological Distance 10
92. Frequency of C - N at Topological Distance 10
93. Frequency of C - O at Topological Distance 10
94. Frequency of C - S at Topological Distance 10
95. Frequency of N - N at Topological Distance 10
96. Frequency of N - O at Topological Distance 10
97. Frequency of N - S at Topological Distance 10
98. Frequency of O - O at Topological Distance 10
99. Frequency of O - S at Topological Distance 10
100. Frequency of S - S at Topological Distance 10

Full Descriptor File (Downloadable EXCEL File)

Chemical Identifiers

1. InChI
2. InChIKey
3. SMILES String
4. IUPAC Name
5. Other Names (Synonyms) or Registry Numbers